Supporting Information

A Computational Study of Acid Catalyzed Aerosol Reactions of Atmospherically Relevant Epoxides

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Contents

1. Theory

Equation 1 of the main text illustrates that $\Delta G^{o}_{act}(T)$ is fundamental to computing a rate constant and requires that the free energy surface (FES) of a solute/solvent system is properly defined. The solvation of a solute may be approximated using either explicit (discreet) or implicit (continuum) solvation models.[1] In explicit solvation models, solute and solvent molecules are both included in calculations in order to account for specific solute-solvent interactions. However, accounting for all intra- and intermolecular interactions accurately may be computationally costly due to the large number of degrees of freedom.[2] Alternatively, implicit solvation models remove explicit solvent degrees of freedom by modeling the solvent as a continuous homogeneous and isotropic medium characterized by a dielectric constant ϵ.[3-5] This model may be hampered by first solvation shell effects that are sensitive to the size of the solute cavity and specific intermolecular interactions such as hydrogen bonding.[6] Hybrid models that incorporate some explicit solvent molecules around a solute (thereby forming a supersolute) immersed in a solvent bath continuum are appealing because they may avoid the disadvantages of either purely explicit or implicit models.[7] In this work, a hybrid model was used to describe a variety of epoxide ring opening reactions in the condensed phase which is described in detail in the computational methods section.

When a continuum model is used, the FES or statistical mechanical potential of mean force,[8] $W(\boldsymbol{R})$ for an N atom solute (or supersolute) with fixed 3N-6 nuclear coordinates at $\boldsymbol{R}$ is given by,

$$W(\boldsymbol{R}) = V(\boldsymbol{R}) + \Delta G^{*}_{S}(\boldsymbol{R}) \tag{S1}$$

where $V(\boldsymbol{R})$ denotes the gas phase potential energy surface and $\Delta G^{*}_{S}(\boldsymbol{R})$ is the free energy of solvation with nuclei clamped and fixed standard state concentrations. The choice of a particular standard state is made by computational convenience or by following convention (standard state solute concentrations of 1 mol/L are used in this work). While $\Delta G^{*}_{S}(\boldsymbol{R})$ depends on the choice of standard state, the rate

constant does not because the standard state concentrations also appear in the denominator of the pre-exponential term in Equation 1 which has a cancelling effect as will be shown in the discussion that follows.

A hierarchy of theoretical treatments exists in finding minima and saddle points on the liquid phase FES. The simplest and most approximate method is deemed the separable-equilibrium solvation (SES) approximation where stationary and saddle points are found on $V(\boldsymbol{R})$ which are then solvated.[9] Free energies in the gas phase are trivial to calculate within the rigid-rotor and harmonic oscillator approximations.[8] In this manner, gas phase reaction and solvation free energies have been combined in thermodynamic cycles invoking the SES to calculate pK_a's of different acids.[10] Another treatment denoted the equilibrium solvation path (ESP) method optimizes structures on $W(\boldsymbol{R})$ in the presence of equilibrium solvation forces from a continuum model.[11] ESP may be further extended by including additional solvent degrees of freedom into $\boldsymbol{R}$ thereby taking into account nonequilibrium solvation (NES) contributions.[12] This extension may be necessary given that solvents do not respond infinitely fast to changes along a reaction coordinate. All calculations in this work were carried out using the ESP method and NES effects were not considered.

It is important to understand that the FES from Equation 2 pertains to solutes with fixed nuclei at $\boldsymbol{R}$. According to Ben-Naim,[13, 14] an additional entropy term to the molar Gibbs free energy (chemical potential) is required to allow the species to move around in the solution volume. The molar Gibbs free energy of a species i in solution may be expressed as,

$$G_i = G_i^* - TS_{lib,i} \tag{S2}$$

The first term G_i^* is the chemical potential of a species with fixed nuclei in solution (pseudochemical potential). The second term has been called the liberation free energy[13] and contains the absolute temperature T and the entropy of liberation $S_{lib,i}$ for species i,

$$S_{lib,i} = -R\ln\left(C_i N_{\mathrm{A}} \Lambda_i^3\right) \tag{S3}$$

where R is the gas constant, C_i is the concentration of i in moles per unit volume, N_{A} is Avogadro's number and Λ_i is the thermal de Broglie wavelength defined by,

$$\Lambda_i = h(2\pi m_i k_B T)^{-1/2} \tag{S4}$$

in which m_i is the mass of species i. The $\Delta G_{act}^{o}(T)$ may now be computed using Equations 3 – 5 and the following,

$$\Delta G_{act}^{o}(T) = \Delta G_{act}^{*}(T) - T\Delta S_{lib,act}(T) \tag{S5}$$

where $\Delta G_{act}^{*}(T)$ is the difference in internal free energy between the transition state and reactant complexes (pseudochemical potential energy difference). In the calculations presented, $\Delta G_{act}^{*}(T)$ is approximated using the zero point inclusive electronic energies with vibrational frequencies calculated in solution using a continuum model.[11] $\Delta S_{lib,act}$ is the difference in liberation entropy between the transition state and separate reactant species. It contains the standard state concentrations (see Equation 4) which cancel the concentration term in the denominator of Equation 1 so that the rate constant does not depend on the choice of standard state. Equations 1 and 6 provide a means to estimate liquid phase rate constants for atmospherically relevant epoxide reactions.

References

1. R. H. Zhou, *Proteins-Structure Function and Genetics*, 2003, **53**, 148-161.
2. R. Iftimie, P. Minary and M. E. Tuckerman, *Proceedings of the National Academy of Sciences of the United States of America*, 2005, **102**, 6654-6659.
3. S. Miertus, E. Scrocco and J. Tomasi, *Chemical Physics*, 1981, **55**, 117-129.
4. J. Tomasi, B. Mennucci and R. Cammi, *Chemical Reviews*, 2005, **105**, 2999-3093.
5. J. Tomasi and M. Persico, *Chemical Reviews*, 1994, **94**, 2027-2094.
6. C. J. Cramer and D. G. Truhlar, *Chemical Reviews*, 1999, **99**, 2161-2200.
7. C. P. Kelly, C. J. Cramer and D. G. Truhlar, *Journal of Physical Chemistry A*, 2006, **110**, 2493-2499.
8. D. A. McQuarrie, *Statistical Mechanics*, Harper & Row, New York, 1973.

9. Y. Y. Chuang, C. J. Cramer and D. G. Truhlar, *International Journal of Quantum Chemistry*, 1998, **70**, 887-896.
10. J. R. Pliego, *Chemical Physics Letters*, 2003, **367**, 145-149.
11. Y. Kim, J. R. Mohrig and D. G. Truhlar, *Journal of the American Chemical Society*, 2010, **132**, 11071-11082.
12. G. Vanderzwan and J. T. Hynes, *Journal of Physical Chemistry*, 1985, **89**, 4181-4188.
13. A. Bennaim, *Journal of Physical Chemistry*, 1978, **82**, 792-803.
14. A. Bennaim and Y. Marcus, *Journal of Chemical Physics*, 1984, **81**, 2016-2027.

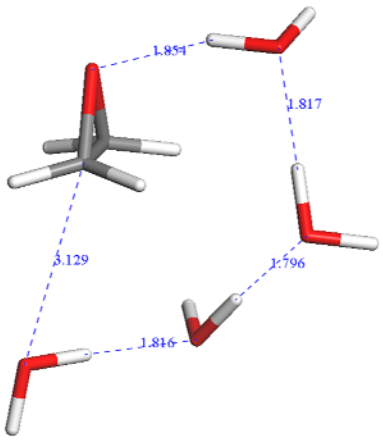
2. Movies of Oxirane Hydrolysis

Attached are three movie files of oxirane hydrolysis using three different acids: H_2O (neutral), H_3O^+ and HCOOH. These movies were constructed using the minimum energy pathway obtained from a nudged elastic band (NEB) calculation at the M062x/6-31+G* level of theory. Intermolecular distances are in units of Angstroms.

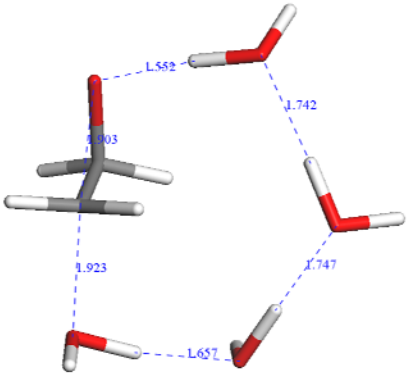
3. Structures, Coordinates and Zero Point Corrected Energies of Reactive Epoxides (all calculations in water continuum unless indicated otherwise)

1. Oxirane hydrolysis (4 H_2O)

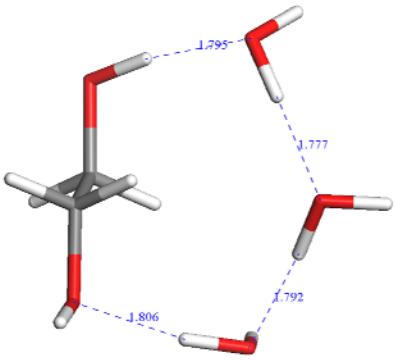
Reactants



Transition State



Products



Reactants			
C	-1.077946	-0.182978	-0.113628
C	0.154063	-0.869798	0.271066
H	0.336992	-1.078515	1.320133
H	-1.468437	-0.311475	-1.115547
H	-1.788337	0.099602	0.656639
H	0.656847	-1.504893	-0.449161
O	0.169206	0.527543	-0.057166
O	-0.085454	1.464335	2.556339
H	0.761830	1.402987	3.011589
H	0.125947	1.323697	1.616098
H	-2.222026	-2.913783	0.192027
O	-2.623619	-2.840678	-0.694659
H	-3.139079	-3.647456	-0.794496
H	-1.712805	-0.778061	4.149095
O	-1.748971	-0.689021	3.190448
H	-1.147206	0.051596	2.978191
H	-1.538267	-2.244364	2.317677
O	-1.508402	-3.103393	1.851105
H	-0.570682	-3.307397	1.764488

G^*_{ZPE} = -459.38311 Hartrees

0 imaginary frequencies

Transition State			
C	-1.121983	-0.528724	-0.298165
C	0.232723	-0.913740	0.081189
H	0.343106	-1.328833	1.087722
H	-1.294280	-0.257495	-1.328935
H	-1.743230	-0.075786	0.463175
H	0.780453	-1.508833	-0.652239
O	0.466897	0.475484	-0.002631
O	-0.050464	1.354700	2.347491
H	0.777752	1.466423	2.825224
H	0.204833	1.048943	1.415908
H	-2.145568	-2.498000	0.472344
O	-2.198784	-2.115449	-0.444158
H	-3.118816	-1.848743	-0.574240
H	-1.361800	-0.733656	4.301727
O	-1.623054	-0.614723	3.382307
H	-1.030826	0.087802	3.031326
H	-1.720335	-2.138299	2.533517
O	-1.860626	-2.972319	2.034056
H	-1.016819	-3.436899	2.071806

G^*_{ZPE} = -459.33705 Hartrees

*i*680.24 cm^{-1}

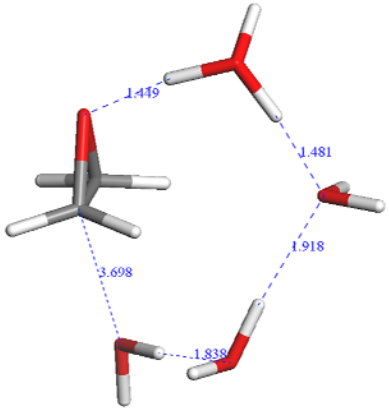
Products			
C	-1.353126	-0.568915	-0.303991
C	0.091520	-0.994733	-0.116430
H	0.178058	-1.624948	0.777413
H	-1.443828	0.046709	-1.203146
H	-1.688773	0.013726	0.561364
H	0.415144	-1.579655	-0.979884
O	0.940893	0.137542	-0.021741
O	0.214828	1.137129	2.449319
H	0.906791	1.090419	3.118033
H	0.753583	0.564785	0.835978
H	-2.012150	-2.638090	1.134466
O	-2.136639	-1.757888	-0.437737
H	-3.050302	-1.507926	-0.616487
H	-1.813203	-0.647952	4.278253
O	-1.821496	-0.499974	3.326398
H	-0.492771	0.542246	2.772191
H	-1.832064	-1.393036	2.926624
O	-1.890864	-2.955584	2.050374
H	-1.007150	-3.339805	2.062080

G^*_{ZPE} = -459.41394 Hartrees

0 imaginary frequencies

2. Oxirane hydrolysis (H_3O^+, 3 H_2O)

Reactants



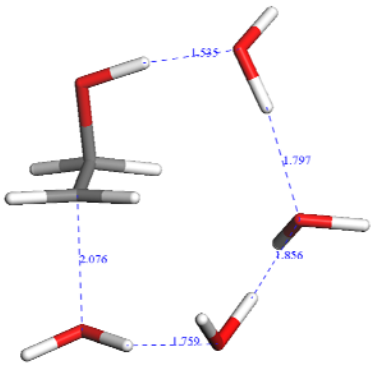
Reactants

C	-1.891892	-0.838792	0.981902
C	-0.656746	-0.954117	0.210521
H	0.201887	-1.437209	0.664902
H	-2.837504	-0.719409	0.468931
H	-0.692310	-0.918185	-0.870130
O	-1.012759	0.301266	0.836833
H	1.159435	0.952472	2.800554
O	0.331671	0.461420	2.921161
H	0.556666	-0.533509	3.101416
H	-0.219053	0.493157	2.034025
H	-0.673423	-3.846469	0.220647
O	-0.452294	-3.785214	-0.726618
H	-0.481785	-4.692643	-1.045982
H	-1.941725	-3.604016	2.166672
O	-1.026863	-3.871477	2.024426
H	-0.495394	-3.179361	2.451230
H	1.599978	-2.247788	2.820346
O	0.775705	-1.989961	3.256136
H	0.886188	-2.237823	4.184460
H	-1.920945	-1.234417	1.990938

G^*_{ZPE} = -459.80205 Hartrees

0 imaginary frequencies

Transition State



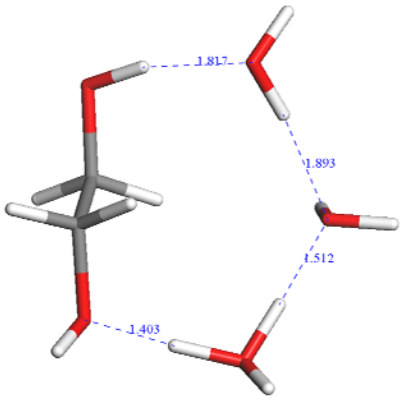
Transition State

C	-1.479228	-0.516523	0.283973
C	-0.160974	-0.007187	-0.040317
H	0.689712	-0.436151	0.480780
H	-2.320911	-0.225468	-0.325651
H	-1.647028	-0.932627	1.268991
H	0.035183	0.266190	-1.070461
O	-0.770288	1.089737	0.683905
H	-0.495784	1.003620	1.660447
O	-1.542300	-2.439934	-0.494599
H	-2.257772	-2.499549	-1.139773
H	0.705006	1.003156	3.381184
O	-0.132407	0.615888	3.100324
H	0.015274	-0.352053	3.074674
H	-1.831731	-2.963867	0.285254
H	-2.908750	-3.198916	2.285120
O	-2.092702	-3.559405	1.920191
H	-1.375665	-3.064316	2.357322
H	0.693879	-2.253578	1.986687
O	0.163850	-2.119061	2.783093
H	0.660543	-2.551776	3.489127

G^*_{ZPE} = -459.77756 Hartrees

*i*604.66 cm^{-1}

Products



Products

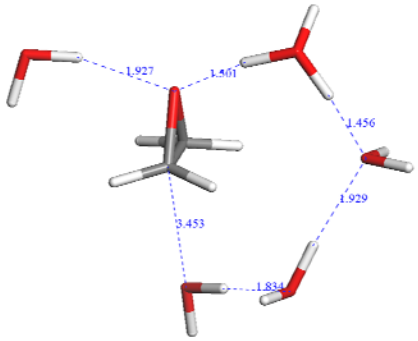
C	-1.949323	0.292029	-0.047695
C	-0.437160	0.195025	-0.136309
H	-0.095537	-0.715369	0.371774
H	-2.312825	1.149667	-0.614651
H	-2.270602	0.381857	0.994448
H	-0.133508	0.138107	-1.183048
O	0.164596	1.348186	0.426825
H	0.034917	1.290851	1.391749
O	-2.491803	-0.915316	-0.617831
H	-3.421648	-0.780251	-0.842222
H	0.366427	0.949120	3.700892
O	-0.353042	0.764014	3.087332
H	-0.380065	-0.204928	3.013799
H	-2.362071	-1.990528	0.274306
H	-3.031782	-2.973125	1.429351
O	-2.201468	-2.779725	0.967777
H	-1.497123	-2.501020	1.660052
H	0.445173	-2.226539	2.240128
O	-0.424211	-2.057424	2.629028
H	-0.443949	-2.565257	3.451655

G^*_{ZPE} = -459.83407 Hartrees

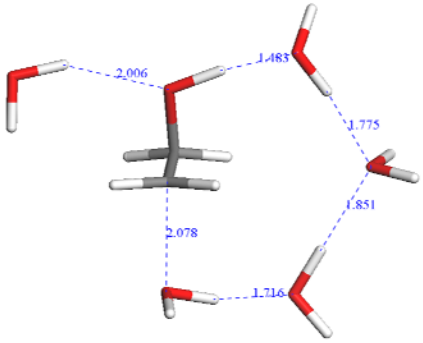
0 imaginary frequencies

3. Oxirane hydrolysis (H_3O^+, 4 H_2O)

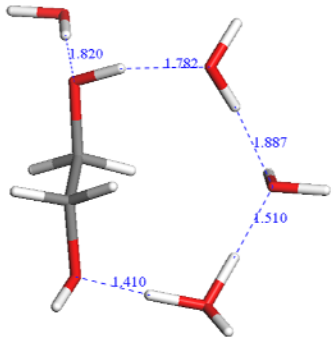
Reactants



Transition State



Products



Reactants

C	-1.771355	-0.720048	1.039845
C	-0.52867	-0.721169	0.272735
H	0.334813	-1.247258	0.665257
H	-2.712498	-0.543015	0.533282
H	-0.558598	-0.541623	-0.794531
O	-0.90337	0.439538	1.056176
H	1.240429	0.887408	3.160823
O	0.403770	0.398587	3.209487
H	0.613777	-0.620178	3.299780
H	-0.110734	0.522536	2.328229
H	-0.908789	-3.588604	0.092102
O	-0.894234	-3.457659	-0.873775
H	-0.876046	-4.347063	-1.241025
H	-1.880062	-3.619337	2.177538
O	-0.978640	-3.829989	1.908701
H	-0.423938	-3.191010	2.384864
H	1.662358	-2.276638	2.892655
O	0.824622	-2.060213	3.325650
H	0.904412	-2.398310	4.228482
H	-1.808254	-1.245413	1.987213
H	-2.639162	1.329450	-1.315602
O	-2.229885	2.086184	-0.882287
H	-1.720843	1.693674	-0.157355

G^*_{ZPE} = -536.21732 Hartrees

0 imaginary frequencies

Transition State

C	-1.427475	-0.075849	0.361585
C	-0.002114	-0.323837	0.242457
H	0.433042	-1.0884	0.879953
H	-1.907842	0.568475	-0.358765
H	0.445048	-0.245608	-0.742448
O	-0.073936	0.971416	0.88883
H	0.914759	0.766737	3.752851
O	0.082801	0.494713	3.347359
H	0.051614	-0.482822	3.420307
H	0.029459	0.835898	1.905296
H	-1.990903	-2.442875	0.017216
O	-2.340466	-1.710237	-0.541112
H	-3.284673	-1.656226	-0.347516
H	-1.573443	-4.284005	1.337225
O	-1.100211	-3.501879	1.032769
H	-0.777500	-3.064539	1.841983
H	0.791686	-2.631064	3.452862
O	-0.090992	-2.251087	3.355834
H	-0.580914	-2.568629	4.125148
H	-1.919029	-0.298748	1.298463
H	-0.657260	1.903278	-1.899436
O	-0.244663	2.660097	-1.468707
H	-0.066207	2.346323	-0.571944

G^*_{ZPE} = -536.19397 Hartrees

*i*606.47 cm^{-1}

Products

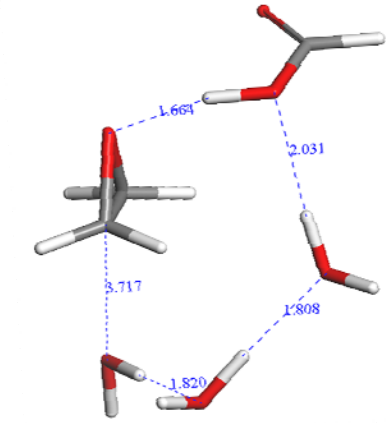
C	-2.016031	0.366474	-0.003042
C	-0.500973	0.41372	-0.044154
H	-0.086098	-0.48732	0.423197
H	-2.441589	1.216436	-0.537416
H	-2.371607	0.370708	1.031505
H	-0.156281	0.45669	-1.07865
O	-0.035940	1.583111	0.615155
H	-0.173872	1.443625	1.573988
O	-2.427673	-0.852896	-0.649447
H	-3.365226	-0.796664	-0.876549
H	0.176749	1.003452	3.824608
O	-0.517517	0.784115	3.193359
H	-0.444478	-0.176351	3.059102
H	-2.194208	-1.964411	0.186854
H	-2.777765	-3.082204	1.258343
O	-1.963907	-2.772629	0.832159
H	-1.305217	-2.469528	1.559547
H	0.588428	-2.111804	2.253692
O	-0.310192	-1.999727	2.593389
H	-0.351420	-2.530852	3.400517
H	2.752416	2.211691	-0.833662
O	2.680044	1.706950	-0.017541
H	1.731418	1.725832	0.205223

G^*_{ZPE} = -536.25111 Hartrees

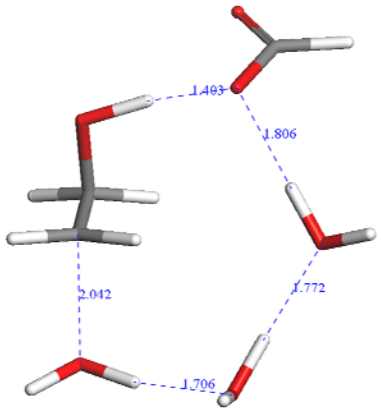
0 imaginary frequencies

4. Oxirane hydrolysis (HCOOH, 3 H_2O)

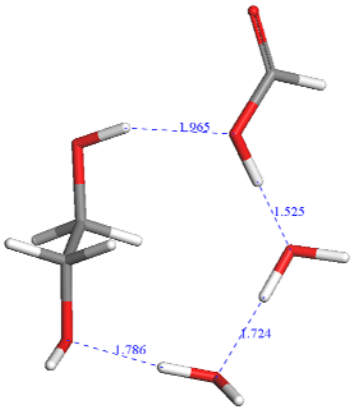
Reactants



Transition State



Products



Reactants

C	-1.746200	-0.912191	1.095815
C	-0.519897	-0.968871	0.301335
H	0.403138	-1.292735	0.773111
H	-2.706721	-0.984760	0.599947
H	-0.584273	-1.075958	-0.774020
O	-1.017144	0.290918	0.791295
C	1.824738	0.832854	2.479422
O	0.583903	0.576566	2.869186
H	-0.038948	0.641776	2.091143
H	-0.834802	-3.924565	0.171113
O	-0.553811	-3.901788	-0.763050
H	-0.449520	-4.826671	-1.008112
H	-2.211410	-3.618594	2.024668
O	-1.327256	-3.987714	1.921830
H	-0.738423	-3.383641	2.414541
H	0.450442	-1.428951	3.162348
O	0.497602	-2.388336	3.281309
H	0.485732	-2.519200	4.236264
H	-1.710607	-1.192407	2.143232
O	2.137044	1.134462	1.352062
H	2.537530	0.738434	3.305208

G^*_{ZPE} = -572.69717 Hartrees

0 imaginary frequencies

Transition State

C	-1.596106	-0.332176	0.294125
C	-0.275975	0.163347	-0.047710
H	0.576744	-0.346276	0.395366
H	-2.451948	0.050337	-0.240872
H	-0.112401	0.497467	-1.066355
O	-0.794707	1.218516	0.786543
C	1.319563	0.911151	3.155152
O	0.085940	0.604285	2.998120
H	-0.423669	1.036671	1.764416
H	-1.862054	-2.766011	0.126663
O	-1.783638	-2.141470	-0.634630
H	-2.636068	-2.164667	-1.087036
H	-2.726354	-3.642158	1.997953
O	-1.846491	-3.614442	1.606353
H	-1.306921	-3.074970	2.220863
H	-0.166108	-1.172886	3.198970
O	-0.210422	-2.146800	3.258411
H	-0.335498	-2.338171	4.194381
H	-1.735937	-0.805461	1.257343
O	1.979329	1.638586	2.408647
H	1.801472	0.470838	4.044292

G^*_{ZPE} = -572.66331 Hartrees

*i*637.16 cm^{-1}

Products

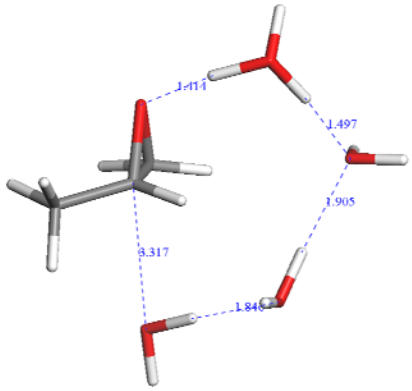
C	-2.036471	0.369868	-0.188627
C	-0.527212	0.230450	-0.121912
H	-0.259226	-0.634200	0.496712
H	-2.302872	1.232013	-0.805468
H	-2.446591	0.512609	0.817314
H	-0.128374	0.071646	-1.125513
O	0.065316	1.417004	0.387647
H	-0.072229	1.414010	1.345073
O	-2.547516	-0.832198	-0.769841
H	-3.488869	-0.718775	-0.942647
C	0.676101	0.923157	3.944530
O	-0.268597	0.557518	3.102658
H	-2.304667	-2.167356	0.391355
H	-2.943843	-3.038626	1.493773
O	-2.103121	-2.850199	1.062156
H	-0.940168	-2.295953	2.207279
H	-0.293076	-0.457570	3.005880
O	-0.258952	-1.973284	2.841581
H	-0.434088	-2.429206	3.673124
O	0.915715	2.085413	4.183620
H	1.225548	0.094714	4.410731

G^*_{ZPE} = -572.72951 Hartrees

0 imaginary frequencies

5. 1,2-epoxypropane hydrolysis (H_3O^+, 3 H_2O)

Reactants



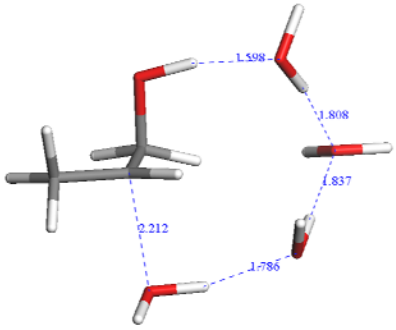
Reactants

C	-1.716832	-0.816314	0.597024
C	-0.338260	-0.968325	0.134978
H	0.375640	-1.511084	0.746147
H	-0.124724	-0.888588	-0.923949
O	-0.772662	0.285528	0.722932
H	0.765240	1.010511	3.167258
O	0.083464	0.333876	3.035098
H	0.499154	-0.598484	3.170502
H	-0.281122	0.390802	2.044852
H	-0.963669	-3.729131	0.205371
O	-0.984616	-3.748786	-0.768737
H	-1.039297	-4.684115	-0.990835
H	-1.819568	-3.460213	2.351482
O	-0.954888	-3.761734	2.050800
H	-0.322714	-3.144688	2.455527
H	1.820640	-2.140006	2.837489
O	0.970547	-2.015346	3.281444
H	1.114735	-2.279638	4.200183
H	-1.957563	-1.245531	1.565372
C	-2.850614	-0.582878	-0.348318
H	-3.585803	0.092271	0.093481
H	-3.342487	-1.534827	-0.559271
H	-2.486376	-0.158141	-1.285306

G^*_{ZPE} = -499.08620 Hartrees

0 imaginary frequencies

Transition State



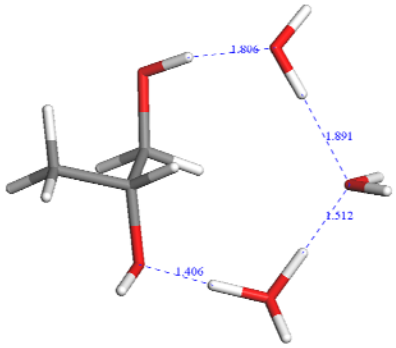
Transition State

C	-1.831112	-0.284744	0.016482
C	-0.378477	-0.335076	0.066982
H	0.068036	-1.074253	0.727779
H	0.141914	-0.214417	-0.877983
O	-0.578248	0.942104	0.712807
H	-0.147910	0.719778	3.813670
O	-0.561118	0.130900	3.171429
H	0.002271	-0.667278	3.144275
H	-0.573116	0.758596	1.701796
H	-1.965881	-2.759455	0.248327
O	-2.115323	-2.377113	-0.642253
H	-3.049256	-2.524314	-0.835798
H	-2.217118	-2.404111	2.454791
O	-1.636611	-3.014437	1.985408
H	-0.736997	-2.764865	2.264548
H	1.616940	-2.192984	2.231090
O	0.903164	-2.211886	2.880120
H	1.267095	-2.660673	3.652571
H	-2.353151	-0.560179	0.926165
C	-2.573191	0.406779	-1.055975
H	-2.963019	1.349724	-0.665742
H	-3.437630	-0.201115	-1.328554
H	-1.947555	0.590195	-1.928101

G^*_{ZPE} = -499.06383 Hartrees

*i*511.18 cm^{-1}

Products



Products

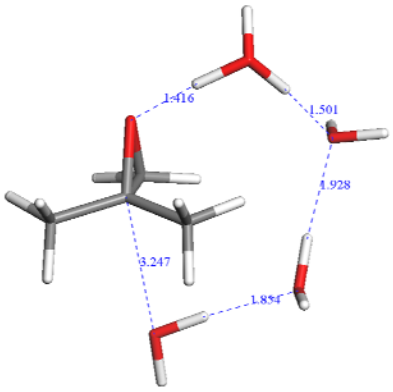
C	-2.019340	0.256148	-0.107330
C	-0.508801	0.202409	-0.294537
H	-0.116661	-0.708933	0.173794
H	-2.248600	0.313837	0.962730
H	-0.279388	0.166566	-1.362563
O	0.115339	1.354850	0.241800
H	0.055426	1.285734	1.213406
O	-2.513055	-1.010452	-0.608945
H	-3.476841	-0.970057	-0.682758
H	0.612126	0.957137	3.466779
O	-0.189394	0.837867	2.945475
H	-0.350742	-0.120645	2.948654
H	-2.150870	-2.097811	0.205223
H	-2.582282	-3.446012	1.070152
O	-1.821182	-2.901698	0.816061
H	-1.375568	-2.542015	1.667261
H	0.193930	-2.396981	2.972307
O	-0.675378	-1.982207	2.884392
H	-1.151142	-2.211734	3.694629
C	-2.671897	1.396541	-0.855220
H	-3.755322	1.376186	-0.714673
H	-2.448860	1.325502	-1.922800
H	-2.297955	2.349841	-0.478936

G^*_{ZPE} = -499.11641 Hartrees

0 imaginary frequencies

6. 2-methyl-1,2-epoxypropane hydrolysis (H_3O^+, 3 H_2O)

Reactants



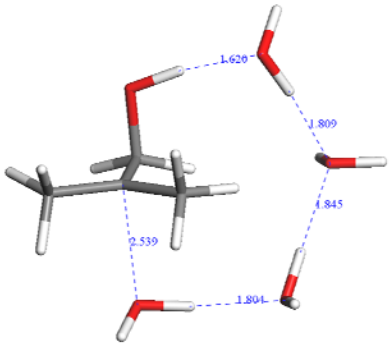
Reactants

C	-1.826169	-0.754509	0.571840
C	-0.425873	-0.981853	0.210026
H	0.195892	-1.593482	0.857258
H	-0.113944	-0.887310	-0.823303
O	-0.816767	0.281213	0.810445
H	0.860292	1.053747	3.120483
O	0.173124	0.370883	3.071927
H	0.606362	-0.553481	3.206204
H	-0.272915	0.387634	2.114008
H	-0.976976	-3.797419	0.321324
O	-1.281452	-3.732988	-0.602056
H	-1.336537	-4.646594	-0.901126
H	-1.301153	-4.032457	2.554669
O	-0.459839	-4.045496	2.083926
H	0.043540	-3.308986	2.468242
H	1.992303	-2.034402	2.890565
O	1.126582	-1.957638	3.315067
H	1.267076	-2.212870	4.237080
C	-2.813204	-0.382489	-0.495825
H	-3.574567	0.287210	-0.089391
H	-3.308166	-1.287435	-0.855373
H	-2.314698	0.104109	-1.334932
C	-2.390514	-1.365210	1.824039
H	-3.115775	-0.683929	2.275693
H	-1.603050	-1.586983	2.547326
H	-2.904973	-2.295054	1.570186

G^*_{ZPE} = -538.37024 Hartrees

0 imaginary frequencies

Transition State



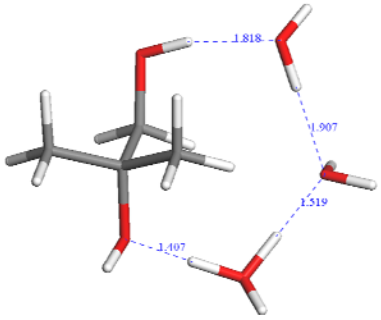
Transition State

C	-1.898437	-0.084176	0.171993
C	-0.439285	-0.182843	0.068947
H	0.024358	-0.931570	0.709670
H	-0.039217	-0.174969	-0.940133
O	-0.397614	1.136571	0.640680
H	0.709404	1.082753	3.568361
O	-0.056885	0.641123	3.184318
H	0.161001	-0.312214	3.191797
H	-0.257889	1.036344	1.626243
H	-1.698960	-2.890744	0.015425
O	-1.850228	-2.417936	-0.827045
H	-2.777229	-2.573717	-1.040060
H	-2.212493	-3.499854	2.112303
O	-1.383019	-3.618390	1.635463
H	-0.738177	-3.071163	2.120670
H	1.364650	-2.155053	2.551664
O	0.525792	-2.075813	3.023628
H	0.682382	-2.489010	3.882266
C	-2.662083	0.576217	-0.897366
H	-3.382394	1.284110	-0.484722
H	-3.238238	-0.221471	-1.383089
H	-2.016284	1.042949	-1.638647
C	-2.585504	-0.477291	1.415345
H	-3.018253	0.412926	1.881651
H	-1.932811	-1.001484	2.110556
H	-3.430655	-1.113431	1.131800

G^*_{ZPE} = -538.35486 Hartrees

*i*302.29 cm^{-1}

Products



Products

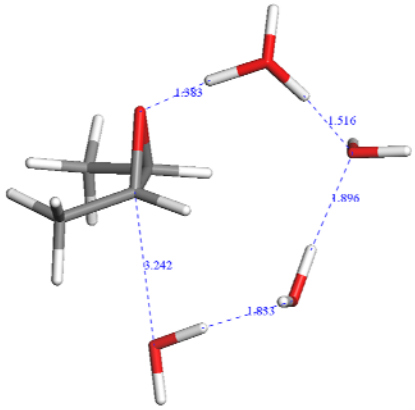
C	-2.092737	0.283709	-0.142182
C	-0.564430	0.193377	-0.112500
H	-0.270576	-0.673665	0.492802
H	-0.200694	0.041989	-1.131742
O	0.029094	1.374720	0.393572
H	0.047457	1.292773	1.364706
O	-2.492935	-1.016557	-0.665403
H	-3.442280	-1.003237	-0.855181
H	0.891976	0.725675	3.497264
O	0.022391	0.698987	3.082642
H	-0.176763	-0.247688	2.985227
H	-2.203013	-2.087363	0.200141
H	-2.762490	-3.265974	1.218712
O	-1.949520	-2.896752	0.841065
H	-1.348907	-2.575340	1.607941
H	0.483795	-2.427274	2.518896
O	-0.412392	-2.120102	2.713526
H	-0.648053	-2.531272	3.556497
C	-2.571810	1.357726	-1.101454
H	-3.663773	1.355712	-1.157193
H	-2.162990	1.189909	-2.100350
H	-2.249146	2.339417	-0.750589
C	-2.676016	0.460871	1.250497
H	-3.767898	0.446347	1.203821
H	-2.362915	1.418920	1.670112
H	-2.337094	-0.339566	1.914113

G^*_{ZPE} = -538.39975 Hartrees

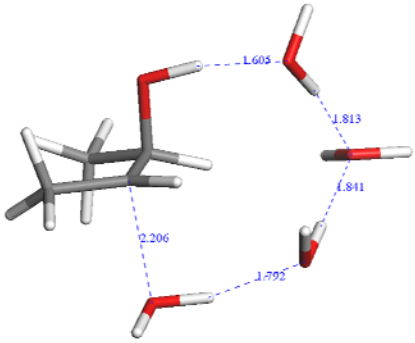
0 imaginary frequencies

7. *cis*-2,3-epoxybutane hydrolysis (H_3O^+, 3 H_2O)

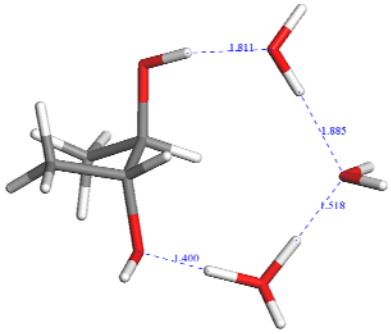
Reactants



Transition State



Products



Reactants			
C	-1.648784	-0.854650	0.520400
C	-0.246559	-0.955997	0.099027
H	0.406219	-1.513832	0.767550
C	-2.797590	-0.601875	-0.403024
C	0.236708	-0.804286	-1.308433
O	-0.736468	0.265609	0.733714
H	1.208975	-0.307560	-1.312216
H	-3.580696	-0.048760	0.118887
H	-3.212830	-1.561217	-0.720212
H	-2.495691	-0.038672	-1.285140
H	-0.455685	-0.224667	-1.917534
H	0.358736	-1.793767	-1.752694
H	0.710783	0.991047	3.204631
O	0.048820	0.299232	3.053132
H	0.485821	-0.616279	3.195797
H	-0.295752	0.350579	2.042013
H	-1.081833	-3.789610	0.282352
O	-1.207661	-3.832810	-0.683421
H	-1.470794	-4.743202	-0.853123
H	-1.770582	-3.481462	2.442836
O	-0.920246	-3.787897	2.108227
H	-0.270502	-3.171386	2.485629
H	1.859639	-2.135586	2.871683
O	1.003958	-2.036346	3.310885
H	1.150303	-2.299565	4.229448
H	-1.895190	-1.344359	1.458950

G^*_{ZPE} = -538.36855 Hartrees

0 imaginary frequencies

Transition State			
C	-1.891195	-0.316969	0.006103
C	-0.430446	-0.294604	0.055137
H	0.001325	-1.031629	0.731144
C	-2.695058	0.315524	-1.063250
C	0.361932	-0.074002	-1.198127
O	-0.718129	0.945446	0.757494
H	1.396030	0.157168	-0.939447
H	-2.740809	1.391561	-0.876284
H	-3.712524	-0.071016	-1.029632
H	-2.255752	0.148578	-2.046010
H	-0.050494	0.748840	-1.783497
H	0.347626	-0.984031	-1.801421
H	-0.230984	0.660570	3.847821
O	-0.632031	0.069655	3.199737
H	-0.030309	-0.697467	3.135157
H	-0.698580	0.730314	1.738631
H	-1.948426	-2.789273	0.199940
O	-2.117277	-2.400351	-0.684133
H	-3.047388	-2.577790	-0.871661
H	-2.191464	-2.479416	2.424395
O	-1.598346	-3.061901	1.935670
H	-0.703367	-2.787757	2.206216
H	1.638911	-2.128092	2.143301
O	0.935368	-2.195517	2.800476
H	1.326804	-2.653674	3.553870
H	-2.382768	-0.637247	0.917097

G^*_{ZPE} = -538.34722 Hartrees

*i*504.92 cm^{-1}

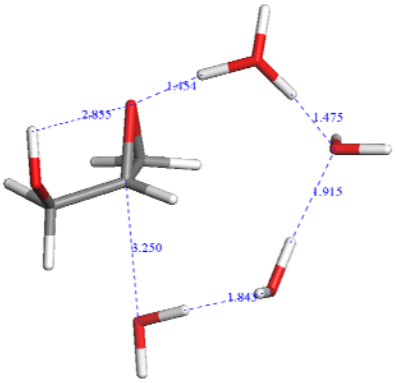
Products			
C	-2.026521	0.343546	-0.096878
C	-0.497975	0.291986	-0.206200
H	-0.166946	-0.607637	0.330653
C	-2.681103	1.436731	-0.912932
H	-2.280947	0.455281	0.962799
C	0.010088	0.243869	-1.632840
O	0.049679	1.443614	0.423399
H	1.089389	0.082436	-1.636117
H	-2.274166	2.408744	-0.628630
H	-3.757624	1.449570	-0.727630
H	-2.511402	1.278964	-1.979802
H	-0.199964	1.184389	-2.147295
H	-0.462432	-0.571073	-2.184473
H	-0.088675	1.341681	1.383869
O	-2.510923	-0.948214	-0.540822
H	-3.477473	-0.929934	-0.575401
H	0.326450	1.017387	3.679881
O	-0.400220	0.802416	3.084622
H	-0.420641	-0.169010	3.050586
H	-2.074571	-2.041998	0.216406
H	-2.416646	-3.467334	1.001343
O	-1.691051	-2.868629	0.767099
H	-1.241189	-2.545806	1.628959
H	0.341855	-2.414607	2.944013
O	-0.548261	-2.041932	2.882306
H	-1.010976	-2.352506	3.672517

G^*_{ZPE} = -538.39701 Hartrees

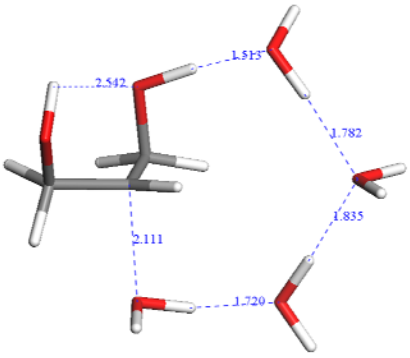
0 imaginary frequencies

8. 2,3-epoxypropan-1-ol hydrolysis (H_3O^+, 3 H_2O) – nucleophile adds to secondary carbon

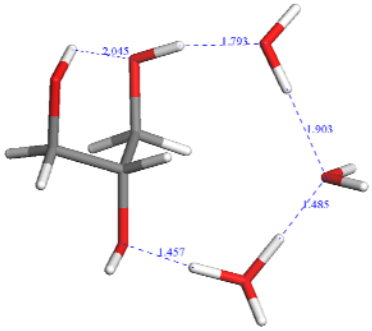
Reactants



Transition State



Products



Reactants

C	-1.631152	-0.797998	0.557479
C	-0.249655	-0.991278	0.124258
H	0.427899	-1.551470	0.760012
H	-0.009193	-0.935416	-0.930478
O	-0.665548	0.278656	0.683089
H	0.828197	1.008333	3.184897
O	0.143719	0.337523	3.036895
H	0.547273	-0.606924	3.178292
H	-0.192397	0.400452	2.052637
H	-1.072996	-3.720322	0.256952
O	-1.121924	-3.744697	-0.716186
H	-1.361416	-4.653661	-0.924740
H	-1.848266	-3.382659	2.413731
O	-1.001207	-3.717884	2.098701
H	-0.341215	-3.114349	2.477924
H	1.838335	-2.150439	2.852693
O	0.990928	-2.008312	3.296820
H	1.130383	-2.269541	4.217341
H	-1.927740	-1.202536	1.521469
C	-2.725556	-0.540182	-0.431567
O	-3.721144	0.320603	0.103064
H	-3.214881	-1.486948	-0.666055
H	-2.300256	-0.126012	-1.350770
H	-3.329685	1.194168	0.220320

G^*_{ZPE} = -574.30311 Hartrees

0 imaginary frequencies

Transition State

C	-1.714979	-0.206507	0.093728
C	-0.304770	-0.406597	-0.197959
H	0.234383	-1.119446	0.420288
H	-0.010737	-0.411456	-1.242673
O	-0.293451	0.935502	0.337938
H	1.131441	0.905312	3.032794
O	0.214806	0.705483	2.808173
H	0.081402	-0.235632	3.045720
H	-0.061282	0.883064	1.331332
H	-1.951747	-2.712566	0.139699
O	-2.460292	-2.105821	-0.447248
H	-3.380637	-2.171934	-0.162818
H	-1.181698	-4.408830	1.477290
O	-0.849894	-3.566364	1.147387
H	-0.645288	-3.039658	1.942363
H	0.581722	-2.339327	3.753840
O	-0.217933	-1.962687	3.364874
H	-0.891639	-2.049722	4.051395
H	-2.035874	-0.361190	1.118393
C	-2.594826	0.610115	-0.810734
O	-3.136312	1.719927	-0.121675
H	-3.433500	-0.006525	-1.130638
H	-2.026175	0.921096	-1.691021
H	-2.410920	2.319451	0.091836

G^*_{ZPE} = -574.27668 Hartrees

*i*574.96 cm^{-1}

Products

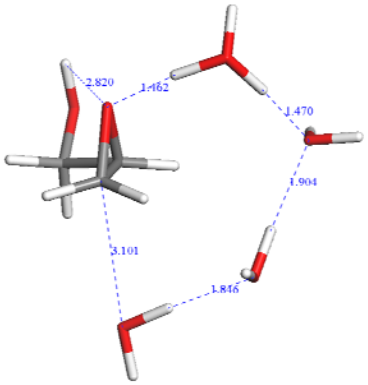
C	-2.007090	0.223618	-0.093353
C	-0.497062	0.116680	-0.268552
H	-0.121506	-0.761684	0.269078
H	-2.258617	0.304830	0.970759
H	-0.271271	-0.003664	-1.330796
O	0.148145	1.299955	0.178672
H	0.135492	1.273857	1.155875
O	-2.549904	-0.999191	-0.622760
H	-3.515808	-0.942221	-0.637747
H	0.700669	0.949242	3.400457
O	-0.107127	0.858351	2.882966
H	-0.310276	-0.091863	2.897705
H	-2.184607	-2.133840	0.215245
H	-2.627709	-3.440715	1.104324
O	-1.862345	-2.910959	0.832008
H	-1.400336	-2.528899	1.674681
H	0.173145	-2.378066	2.934268
O	-0.692605	-1.955154	2.847309
H	-1.160916	-2.157074	3.669470
C	-2.598956	1.410504	-0.844871
H	-3.686434	1.311516	-0.878103
H	-2.218923	1.416148	-1.873318
O	-2.313699	2.637095	-0.188839
H	-1.355156	2.665192	-0.058628

G^*_{ZPE} = -574.33287 Hartrees

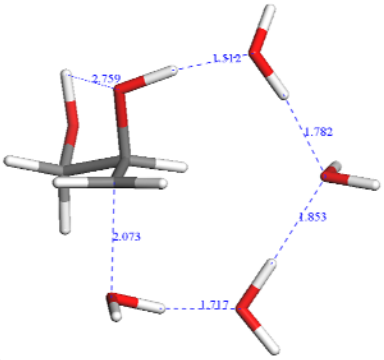
0 imaginary frequencies

9. 2,3-epoxypropan-1-ol hydrolysis (H_3O^+, 3 H_2O) – nucleophile adds to primary carbon

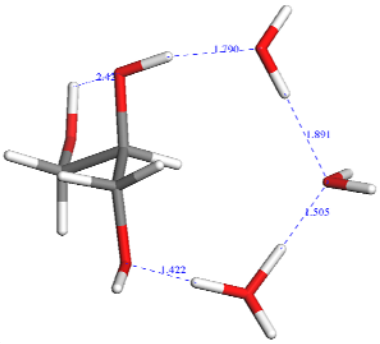
Reactants



Transition State



Products



Reactants

C	-1.635540	-0.947777	0.506444
C	-0.224755	-1.032603	0.137138
H	0.444760	-1.580193	0.796910
H	-2.374193	-0.747701	-0.260615
C	0.221697	-0.848510	-1.280518
O	-0.751161	0.171002	0.754493
O	1.478831	-0.189435	-1.346045
H	-0.541335	-0.294579	-1.835985
H	0.351058	-1.829012	-1.740686
H	0.675330	0.930168	3.279582
O	0.039181	0.215000	3.122239
H	0.518408	-0.697143	3.244966
H	-0.303224	0.272533	2.142703
H	-1.172065	-3.812568	0.377444
O	-1.411913	-3.849111	-0.566283
H	-1.471771	-4.789117	-0.765635
H	-1.666740	-3.501763	2.594695
O	-0.845659	-3.809231	2.194078
H	-0.165849	-3.204992	2.535038
H	1.961800	-2.092553	2.905131
O	1.103346	-2.042079	3.347591
H	1.263262	-2.299864	4.265786
H	-1.975588	-1.448757	1.405501
H	1.358197	0.715666	-1.035872

G^*_{ZPE} = -574.30335 Hartrees

0 imaginary frequencies

Transition State

C	-1.763803	-0.274480	0.192577
C	-0.324584	-0.402385	0.047326
H	0.190026	-1.025375	0.776559
H	-2.320447	0.228129	-0.584257
C	0.269040	-0.442865	-1.331905
O	-0.500040	0.954350	0.533264
O	1.649742	-0.124869	-1.303362
H	-0.281855	0.238156	-1.988263
H	0.175607	-1.458818	-1.718980
H	0.616567	1.165292	3.368010
O	-0.175865	0.729969	3.032188
H	-0.036402	-0.229773	3.175312
H	-0.347008	0.941811	1.545125
H	-2.022649	-2.715392	0.095604
O	-2.515316	-2.085083	-0.479924
H	-3.440254	-2.147557	-0.210223
H	-1.215706	-4.381393	1.462346
O	-0.898687	-3.552508	1.086752
H	-0.579610	-3.028550	1.844491
H	1.087404	-2.190629	3.122568
O	0.143721	-2.002833	3.207131
H	-0.103202	-2.356950	4.070899
H	-2.206794	-0.425417	1.166958
H	1.741204	0.806386	-1.069626

G^*_{ZPE} = -574.28003 Hartrees

*i*600.16 cm^{-1}

Products

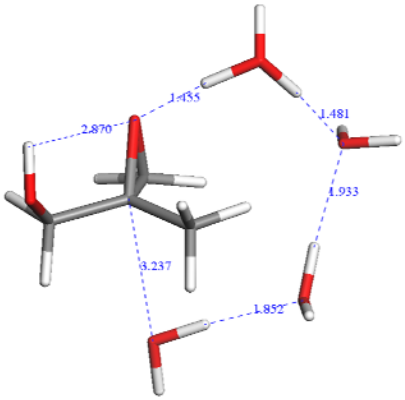
C	-2.022005	0.324945	-0.039789
C	-0.503010	0.290049	-0.101301
H	-0.136372	-0.587822	0.448009
H	-2.407407	1.143011	-0.652659
H	-2.346520	0.460300	0.995268
C	0.004003	0.230645	-1.528008
O	0.009819	1.477465	0.483011
O	1.422509	0.145247	-1.568282
H	-0.342823	1.120574	-2.067150
H	-0.383442	-0.656586	-2.028777
H	-0.033847	1.364658	1.452353
O	-2.525185	-0.922773	-0.550825
H	-3.489496	-0.884753	-0.599802
H	0.534045	0.909526	3.662886
O	-0.261141	0.788202	3.132106
H	-0.372259	-0.175308	3.063509
H	-2.097660	-2.050674	0.201509
H	-2.428286	-3.479465	0.968730
O	-1.710076	-2.867462	0.745709
H	-1.269574	-2.541050	1.615411
H	0.290480	-2.430372	2.931603
O	-0.593023	-2.042562	2.864521
H	-1.066017	-2.346609	3.651423
H	1.769576	0.905219	-1.085789

G^*_{ZPE} = -574.33532 Hartrees

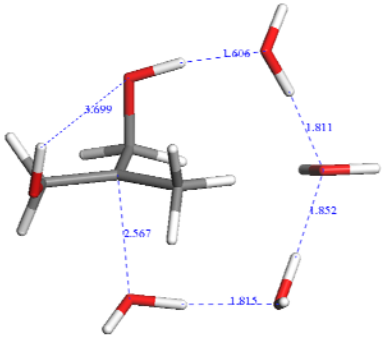
0 imaginary frequencies

10. 2-methyl-2,3-epoxypropan-1-ol hydrolysis (H_3O^+, 3 H_2O)

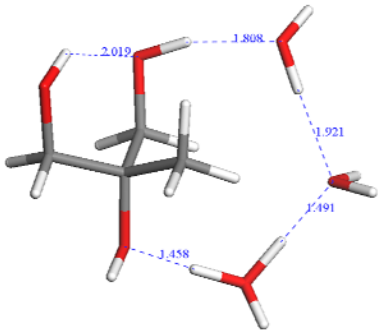
Reactants



Transition State



Products



Reactants			
C	-1.866450	-0.791213	0.546355
C	-0.464867	-1.012322	0.188662
H	0.151466	-1.619268	0.844896
C	-2.825553	-0.437167	-0.560535
H	-0.148705	-0.928884	-0.844402
O	-0.868821	0.251565	0.772509
O	-3.857595	0.432298	-0.119190
H	-3.309360	-1.353124	-0.905210
H	-2.273819	0.005789	-1.394526
H	0.789768	1.040776	3.122611
O	0.102523	0.358177	3.066911
H	0.533713	-0.573663	3.202718
H	-0.328076	0.378465	2.117249
H	-1.023139	-3.824558	0.305795
O	-1.319254	-3.760944	-0.620418
H	-1.380310	-4.675056	-0.916621
H	-1.365705	-4.052907	2.537013
O	-0.520993	-4.062701	2.072302
H	-0.024400	-3.322868	2.458522
H	1.912972	-2.036111	2.891430
O	1.046167	-1.959086	3.314072
H	1.183784	-2.213000	4.237026
C	-2.450828	-1.385160	1.796006
H	-1.667930	-1.608137	2.523438
H	-2.971029	-2.312450	1.543966
H	-3.170501	-0.695516	2.241377
H	-3.460019	1.283709	0.097538

G^*_{ZPE} = -613.58730 Hartrees

0 imaginary frequencies

Transition State			
C	-1.820387	-0.054449	0.222390
C	-0.373200	-0.209158	0.067494
H	0.081824	-0.981643	0.684182
C	-2.563945	0.575584	-0.896380
H	-0.003949	-0.202689	-0.954362
O	-0.278586	1.101356	0.652142
O	-3.877703	0.968443	-0.583758
H	-2.614819	-0.196191	-1.674063
H	-1.961659	1.394791	-1.304154
H	1.006904	0.933220	3.498156
O	0.179958	0.570775	3.159376
H	0.297509	-0.400201	3.164181
H	-0.086956	0.985814	1.630550
H	-1.904870	-2.908790	0.214933
O	-1.933403	-2.464520	-0.655149
H	-2.852950	-2.524967	-0.937390
H	-2.541920	-3.244223	2.337458
O	-1.752425	-3.576735	1.895523
H	-1.014549	-3.093861	2.311086
H	1.159223	-2.345788	2.348556
O	0.455013	-2.196368	2.992419
H	0.769919	-2.610384	3.805768
C	-2.499559	-0.371076	1.484118
H	-1.840341	-0.857450	2.199964
H	-3.348110	-1.018420	1.234705
H	-2.934298	0.542524	1.901886
H	-3.845454	1.776383	-0.057583

G^*_{ZPE} = -613.56887 Hartrees

*i*305.39 cm^{-1}

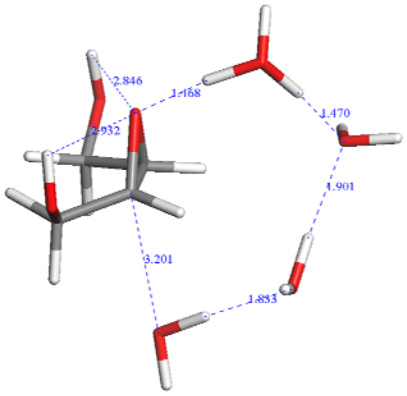
Products			
C	-2.172637	0.333955	-0.061377
C	-0.641187	0.326527	-0.052893
H	-0.282386	-0.505885	0.563828
C	-2.708732	1.427830	-0.989571
C	-2.757505	0.430078	1.336639
H	-0.285396	0.180754	-1.075497
O	-0.118478	1.558033	0.421591
O	-2.531691	2.729931	-0.452460
H	-3.783473	1.281145	-1.128620
H	-2.216978	1.336612	-1.965013
H	-0.057992	1.481844	1.393281
O	-2.524100	-0.936903	-0.658451
H	-3.486481	-0.989850	-0.758105
H	0.872892	0.826041	3.453741
O	-0.011501	0.811029	3.071091
H	-0.223647	-0.132694	2.973113
H	-2.086714	-2.064842	0.154808
H	-2.452985	-3.435122	0.983705
O	-1.718223	-2.854335	0.731446
H	-1.261586	-2.502602	1.589697
H	0.310472	-2.454578	2.874575
O	-0.550388	-2.018487	2.807684
H	-1.030284	-2.273327	3.608162
H	-3.849780	0.422964	1.287904
H	-2.440204	1.353129	1.823846
H	-2.421074	-0.415797	1.941828
H	-1.610314	2.788134	-0.159010

G^*_{ZPE} = -613.61677 Hartrees

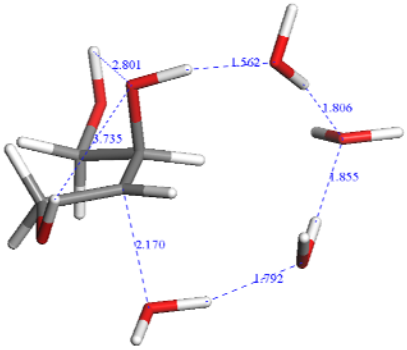
0 imaginary frequencies

11. *cis*-2,3-epoxybutane-1,4-diol hydrolysis (H_3O^+, 3 H_2O)

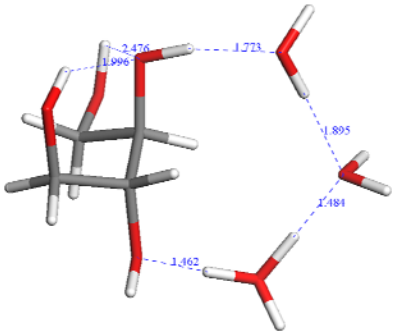
Reactants



Transition State



Products



Reactants

C	-1.679199	-0.854095	0.461496
C	-0.268943	-0.984685	0.084530
H	0.358809	-1.569932	0.754130
C	-2.794064	-0.556189	-0.496706
C	0.271143	-0.819915	-1.305125
O	-0.750858	0.234731	0.710799
O	1.582768	-0.271415	-1.263803
O	-3.859380	0.116433	0.161219
H	-3.193475	-1.503023	-0.863952
H	-2.436589	0.028884	-1.345915
H	-0.385104	-0.196711	-1.915256
H	0.353347	-1.804994	-1.765620
H	0.712156	0.946782	3.234152
O	0.059476	0.246760	3.076616
H	0.514783	-0.678439	3.195356
H	-0.287688	0.318357	2.101706
H	-1.127377	-3.778904	0.353765
O	-1.207481	-3.830788	-0.616564
H	-1.457549	-4.743936	-0.791376
H	-1.804161	-3.393200	2.547113
O	-0.984081	-3.742770	2.180672
H	-0.290381	-3.155010	2.522656
H	1.895067	-2.134919	2.841832
O	1.045535	-2.045454	3.295453
H	1.207167	-2.304909	4.212921
H	-1.984643	-1.352489	1.378233
H	-3.560498	1.005351	0.385357
H	1.516562	0.641349	-0.959741

G^*_{ZPE} = -688.80127 Hartrees

0 imaginary frequencies

Transition State

C	-1.785905	-0.200931	0.052889
C	-0.344758	-0.402461	0.015076
H	0.038558	-1.156961	0.700851
C	-2.541091	0.509227	-1.026236
C	0.391976	-0.364671	-1.296979
O	-0.419837	0.902119	0.645068
O	1.790078	-0.288670	-1.077319
O	-3.922894	0.572205	-0.745858
H	-2.417312	-0.043134	-1.959283
H	-2.105014	1.503082	-1.162494
H	0.047302	0.475368	-1.907015
H	0.194272	-1.294703	-1.832296
H	0.179637	0.760729	3.702980
O	-0.305568	0.183619	3.101826
H	0.191071	-0.658483	3.076791
H	-0.358746	0.742657	1.643959
H	-2.257489	-2.593566	0.377625
O	-2.446075	-2.193754	-0.497811
H	-3.408396	-2.186704	-0.579383
H	-2.230974	-2.204332	2.597217
O	-1.755763	-2.862671	2.077181
H	-0.816432	-2.706652	2.282131
H	1.610018	-2.316261	2.107962
O	0.919200	-2.284475	2.781241
H	1.278921	-2.755604	3.542423
H	-2.279199	-0.391126	0.999308
H	-4.071378	1.239865	-0.065912
H	1.996566	0.589757	-0.737281

G^*_{ZPE} = -688.77749 Hartrees

*i*533.18 cm^{-1}

Products

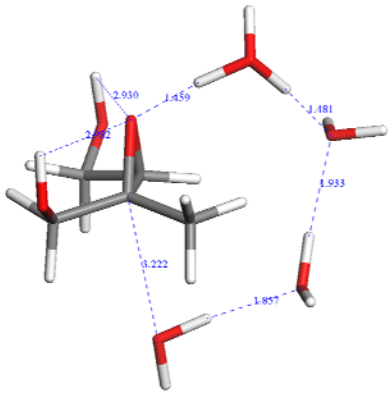
C	-2.079745	0.349489	-0.089261
C	-0.548234	0.311111	-0.131955
H	-0.212972	-0.563791	0.440032
C	-2.706642	1.454914	-0.932631
H	-2.384373	0.475091	0.955814
C	0.026743	0.216885	-1.532191
O	-0.025346	1.497675	0.455944
O	1.430007	-0.011851	-1.482799
O	-2.387510	2.743984	-0.429210
H	-3.793622	1.351947	-0.892797
H	-2.396930	1.350517	-1.978033
H	-0.182046	1.139480	-2.084475
H	-0.416381	-0.623100	-2.067917
H	-0.078472	1.389376	1.427496
O	-2.543631	-0.921178	-0.574028
H	-3.511412	-0.931076	-0.567343
H	0.467040	0.973100	3.637375
O	-0.311086	0.818755	3.090113
H	-0.389831	-0.148533	3.031093
H	-2.060902	-2.068105	0.193562
H	-2.373059	-3.491250	0.950420
O	-1.664396	-2.866512	0.731351
H	-1.228369	-2.528876	1.606523
H	0.318572	-2.395139	2.911131
O	-0.572047	-2.024493	2.838807
H	-1.043043	-2.332430	3.625586
H	-1.448333	2.738089	-0.192008
H	1.823716	0.722204	-0.996169

G^*_{ZPE} = -688.83227 Hartrees

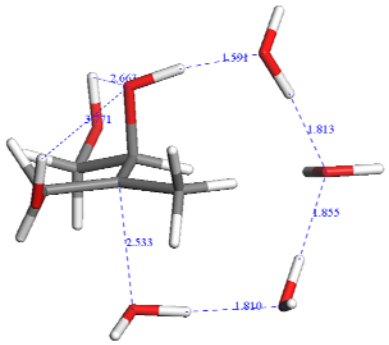
0 imaginary frequencies

12. β-IEPOX hydrolysis (H_3O^+, 3 H_2O) – nucleophile adds to tertiary carbon

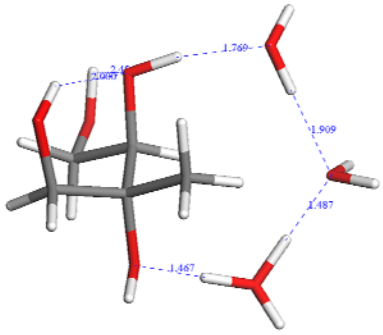
Reactants



Transition State



Products



Reactants

C	-1.822842	-0.759752	0.484594
C	-0.410343	-0.985825	0.148251
H	0.150962	-1.606692	0.845420
C	-2.818117	-0.388561	-0.588510
C	0.197853	-0.888222	-1.220692
O	-0.821881	0.273849	0.747361
O	1.576386	-0.548239	-1.130297
O	-3.920590	0.336215	-0.062910
H	-3.220020	-1.312117	-1.010447
H	-2.334538	0.180576	-1.383624
H	-0.333191	-0.164857	-1.841410
H	0.143635	-1.868033	-1.696294
H	0.735247	1.050056	3.179037
O	0.061284	0.359148	3.080613
H	0.502894	-0.569429	3.209254
H	-0.330418	0.393316	2.115920
H	-1.121104	-3.840895	0.355815
O	-1.500638	-3.797719	-0.540459
H	-1.480572	-4.707681	-0.854685
H	-1.314458	-4.075899	2.568651
O	-0.482126	-4.084303	2.081832
H	0.020221	-3.341223	2.453977
H	1.913274	-1.997499	2.894943
O	1.042740	-1.944116	3.313539
H	1.181579	-2.199968	4.235849
C	-2.396589	-1.389228	1.724979
H	-1.604208	-1.653173	2.427356
H	-2.942546	-2.295270	1.451951
H	-3.090953	-0.700319	2.208759
H	-3.605289	1.203904	0.215759
H	1.642191	0.367026	-0.834591

G^*_{ZPE} = -728.08526 Hartrees

0 imaginary frequencies

Transition State

C	-1.848199	-0.064364	0.200131
C	-0.396880	-0.247022	0.068837
H	0.007306	-0.998305	0.748569
C	-2.606456	0.590106	-0.902612
C	0.260340	-0.303411	-1.289059
O	-0.310513	1.075028	0.640547
O	1.666631	-0.200781	-1.138737
O	-3.944707	0.886192	-0.583692
H	-2.604753	-0.118378	-1.738582
H	-2.053588	1.476452	-1.230022
H	-0.115702	0.489657	-1.940850
H	0.050815	-1.269983	-1.746079
H	0.998164	0.946592	3.459483
O	0.169087	0.573855	3.137117
H	0.300124	-0.395633	3.136828
H	-0.113997	0.973312	1.622915
H	-1.989639	-2.879275	0.182999
O	-2.106172	-2.426715	-0.676078
H	-3.056927	-2.432135	-0.835675
H	-2.474512	-3.286615	2.324010
O	-1.696905	-3.570374	1.829570
H	-0.955284	-3.089529	2.240675
H	1.216245	-2.319578	2.320660
O	0.499610	-2.188052	2.954702
H	0.807474	-2.607545	3.767938
C	-2.523237	-0.375772	1.469699
H	-1.862053	-0.871314	2.177699
H	-3.385300	-1.008593	1.235777
H	-2.933296	0.546495	1.893481
H	-3.969087	1.683963	-0.041416
H	1.873321	0.690558	-0.833637

G^*_{ZPE} = -728.06705 Hartrees

*i*325.98 cm^{-1}

Products

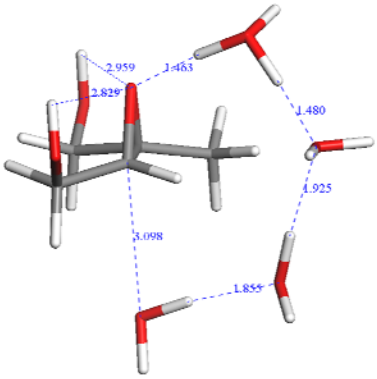
C	-2.165161	0.347672	-0.094337
C	-0.622586	0.353309	-0.069434
H	-0.296891	-0.508052	0.529530
C	-2.746675	1.418480	-1.022863
C	-2.731344	0.454980	1.312375
C	0.020069	0.252958	-1.441840
O	-0.140728	1.554033	0.523185
O	1.424183	0.060889	-1.319631
O	-2.456128	2.736719	-0.582410
H	-3.835015	1.313190	-1.034901
H	-2.381324	1.257299	-2.042375
H	-0.182887	1.165154	-2.013669
H	-0.373323	-0.603074	-1.989550
H	-0.097080	1.413836	1.491085
O	-2.518664	-0.936446	-0.658759
H	-3.481810	-0.990913	-0.751403
H	0.862739	0.798495	3.504076
O	-0.028272	0.770497	3.137591
H	-0.228115	-0.175928	3.039212
H	-2.081130	-2.060323	0.176502
H	-2.467080	-3.420872	1.005567
O	-1.723943	-2.851165	0.752338
H	-1.259371	-2.507294	1.610868
H	0.316608	-2.483745	2.885583
O	-0.544911	-2.047162	2.831324
H	-1.022356	-2.321567	3.626785
H	-3.820348	0.366638	1.276487
H	-2.477410	1.415177	1.763026
H	-2.329094	-0.344519	1.940139
H	-1.541332	2.745123	-0.264105
H	1.773061	0.808836	-0.820106

G^*_{ZPE} = -728.11616 Hartrees

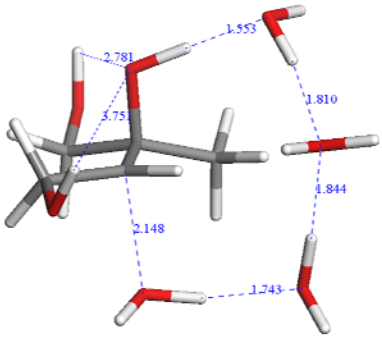
0 imaginary frequencies

13. β-IEPOX hydrolysis (H_3O^+, 3 H_2O) – nucleophile adds to secondary carbon

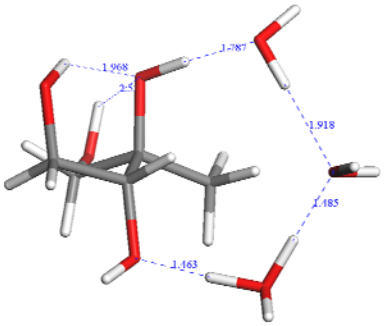
Reactants



Transition State



Products



Reactants

C	-1.471545	-0.729488	0.539548
C	-0.163634	-0.732170	-0.130520
C	1.004388	-1.404530	0.537044
C	-2.811278	-0.573068	-0.118798
H	-1.505974	-1.215168	1.513706
H	0.840086	-1.492953	1.611913
H	1.918105	-0.834606	0.360444
H	1.133896	-2.403723	0.114889
C	-0.061759	-0.567182	-1.627990
O	-0.641957	0.464878	0.559868
O	1.183156	-0.001567	-2.012902
O	-3.707810	0.108527	0.751160
H	-3.232583	-1.563771	-0.293251
H	-2.732875	-0.049354	-1.072539
H	-0.885757	0.039051	-2.007010
H	-0.112890	-1.557564	-2.084582
H	1.207596	0.912290	-1.705518
H	-3.401648	1.018279	0.844506
H	-0.140871	0.700777	1.914140
O	-1.334452	-3.648283	-0.489129
H	-1.607440	-4.561641	-0.624737
H	1.062631	0.972828	2.986884
O	0.111937	0.791193	2.919082
H	-0.086866	-0.114797	3.383535
H	-1.064976	-3.611576	0.446478
H	-1.243912	-4.291022	2.691677
O	-0.601233	-3.734262	2.238004
H	-0.538754	-2.933293	2.783567
H	0.219368	-1.671957	4.654433
O	-0.426394	-1.427292	3.977077
H	-1.278346	-1.385765	4.433333

G^*_{ZPE} = -728.08517 Hartrees

0 imaginary frequencies

Transition State

C	-1.482247	-0.231928	0.140541
C	-0.145106	-0.346218	-0.437015
C	0.747743	-1.438431	0.094100
C	-2.615894	0.527950	-0.482151
H	-1.578339	-0.531604	1.180076
H	0.538593	-1.634573	1.146990
H	1.793602	-1.149265	-0.018207
H	0.572658	-2.351468	-0.478676
C	-0.028026	-0.094899	-1.927337
O	-0.041223	0.917951	0.284292
O	1.320483	0.080857	-2.321715
O	-3.798557	0.406233	0.281066
H	-2.822556	0.116021	-1.471057
H	-2.315047	1.572003	-0.602516
H	-0.626697	0.775770	-2.210180
H	-0.409169	-0.972108	-2.453331
H	1.645982	0.898321	-1.925999
H	-3.705536	0.932668	1.083951
H	0.368890	0.773266	1.202667
O	-2.295069	-2.154449	-0.366800
H	-3.256536	-2.089090	-0.299029
H	1.795236	0.156058	2.575420
O	0.928870	0.576644	2.638239
H	0.345187	-0.092818	3.048550
H	-2.015122	-2.696598	0.405499
H	-1.962967	-4.011382	2.284146
O	-1.341229	-3.425691	1.837887
H	-1.172241	-2.703030	2.470564
H	-0.761648	-1.559238	4.503770
O	-0.919284	-1.265325	3.597713
H	-1.760737	-0.792630	3.631233

G^*_{ZPE} = -728.06311 Hartrees

*i*543.70 cm^{-1}

Products

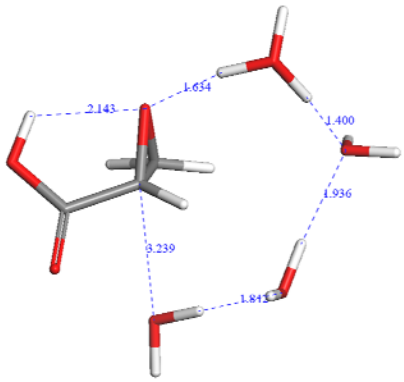
C	-1.793129	0.152218	-0.142090
C	-0.323184	0.071166	-0.609095
C	0.298235	-1.250476	-0.174365
C	-2.558176	1.379876	-0.630747
H	-1.785566	0.150262	0.956163
H	0.130560	-1.409989	0.894052
H	1.372643	-1.231064	-0.359218
H	-0.134629	-2.087456	-0.726210
C	-0.206747	0.283729	-2.115683
O	0.379328	1.166477	-0.010608
O	1.114331	0.063557	-2.590901
O	-2.018286	2.585258	-0.113922
H	-3.587988	1.309816	-0.270975
H	-2.586673	1.395617	-1.725819
H	-0.520235	1.303252	-2.361148
H	-0.854230	-0.421091	-2.639676
H	1.699979	0.666348	-2.117295
H	-1.052565	2.509554	-0.146534
H	0.425232	1.013199	0.956229
O	-2.470238	-1.035308	-0.596351
H	-3.413190	-0.853775	-0.721187
H	1.124514	0.675429	3.174317
O	0.278797	0.737862	2.716249
H	-0.152037	-0.120571	2.864268
H	-2.400284	-2.072806	0.433240
H	-3.194800	-3.042852	1.487601
O	-2.309327	-2.780828	1.191770
H	-1.792154	-2.382552	1.995151
H	-0.267069	-2.404897	3.324484
O	-1.008615	-1.817363	3.122337
H	-1.528774	-1.767999	3.936239

G^*_{ZPE} = -728.11218 Hartrees

0 imaginary frequencies

14. 2,3-epoxypropanoic acid hydrolysis (H_3O^+, 3 H_2O)

Reactants

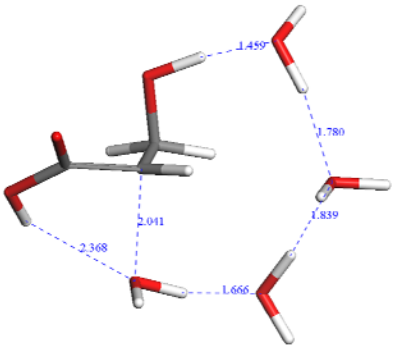


Reactants			
C	-1.656542	-0.770511	0.587867
C	-0.278945	-0.958561	0.112233
H	0.395008	-1.541671	0.730108
H	-0.069865	-0.892387	-0.948758
O	-0.702446	0.285247	0.699584
H	0.896367	1.002301	3.318707
O	0.203687	0.342682	3.155601
H	0.601749	-0.640737	3.238346
H	-0.139520	0.460000	2.223235
H	-1.078110	-3.697068	0.246120
O	-1.122828	-3.682031	-0.727301
H	-1.392127	-4.573096	-0.972920
H	-1.845238	-3.402924	2.415856
O	-0.993926	-3.712093	2.085870
H	-0.344482	-3.096760	2.462240
H	1.848571	-2.116195	2.835893
O	1.003952	-1.981198	3.288955
H	1.140014	-2.277895	4.199954
H	-1.972936	-1.227377	1.518516
C	-2.744822	-0.544296	-0.415287
O	-2.621292	0.522371	-1.199797
O	-3.676314	-1.301730	-0.524913
H	-1.844446	1.048788	-0.945070

G^*_{ZPE} = -648.36333 Hartrees

0 imaginary frequencies

Transition State

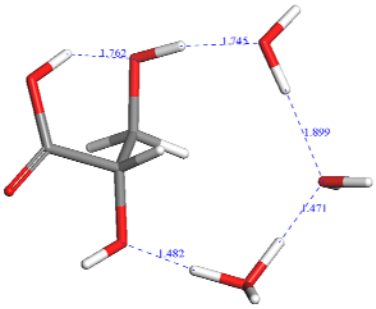


Transition State			
C	-1.564324	-0.128764	0.353057
C	-0.150717	-0.184335	0.016692
H	0.455055	-0.884835	0.583929
H	0.137527	-0.075017	-1.024411
O	-0.300249	1.099601	0.663578
H	1.213338	0.788710	3.244330
O	0.273315	0.682717	3.054498
H	0.074616	-0.271730	3.164278
H	-0.036051	0.995949	1.663888
H	-1.763120	-2.514248	-0.043539
O	-2.360889	-1.830116	-0.445592
H	-3.242186	-1.990956	-0.080567
H	-0.823783	-4.296433	0.901441
O	-0.560648	-3.389614	0.706822
H	-0.476356	-2.951321	1.574878
H	-0.159876	-2.455161	3.846178
O	-0.528029	-1.945418	3.113123
H	-1.470169	-1.869011	3.312640
H	-1.872555	-0.395776	1.356393
C	-2.537713	0.721781	-0.439744
O	-2.509868	0.620285	-1.760664
O	-3.290062	1.473451	0.118887
H	-1.979648	-0.136991	-2.056690

G^*_{ZPE} = -648.32922 Hartrees

*i*615.03 cm^{-1}

Products



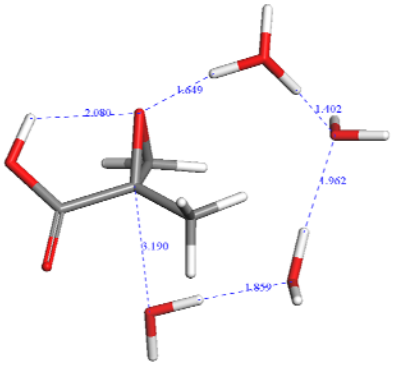
Products			
C	-1.878476	0.118513	-0.195903
C	-0.356497	0.171088	-0.342381
H	0.071698	-0.698458	0.163741
H	-2.139710	0.232570	0.865020
H	-0.083397	0.140088	-1.398343
O	0.139694	1.381928	0.208087
H	0.137194	1.279343	1.185098
O	-2.343380	-1.128958	-0.682878
H	-3.191338	-0.991206	-1.137086
H	0.768973	0.892337	3.357691
O	-0.042483	0.784028	2.849121
H	-0.217165	-0.172171	2.852067
H	-2.389204	-2.149416	0.391092
H	-3.196722	-2.865652	1.610263
O	-2.333995	-2.824857	1.168792
H	-1.620071	-2.504319	1.852230
H	0.266634	-2.455336	2.558102
O	-0.576869	-2.034816	2.776607
H	-0.774984	-2.307671	3.683436
C	-2.578547	1.240437	-0.944431
O	-3.565911	1.037629	-1.612383
O	-2.065050	2.452024	-0.803661
H	-1.205987	2.389660	-0.320126

G^*_{ZPE} = -648.40041 Hartrees

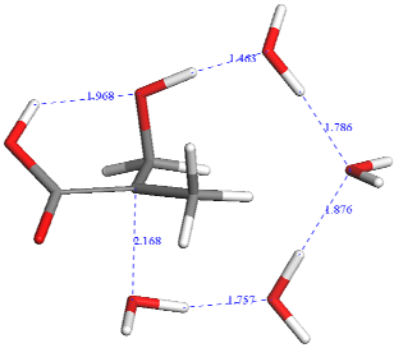
0 imaginary frequencies

15. MAE hydrolysis (H_3O^+, 3 H_2O) – nucleophile adds to tertiary carbon

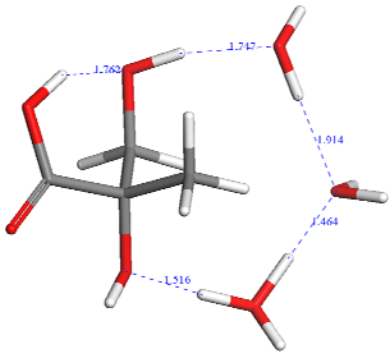
Reactants



Transition State



Products



Reactants

C	-1.832399	-0.786245	0.533267
C	-0.437324	-1.050954	0.146465
H	0.167892	-1.649028	0.819655
C	-2.784582	-0.503570	-0.600208
H	-0.149191	-1.023295	-0.897939
O	-0.828189	0.230532	0.678089
O	-2.470202	0.511927	-1.401101
O	-3.769279	-1.171531	-0.795275
H	0.882971	1.058944	3.193329
O	0.177312	0.398034	3.106087
H	0.575319	-0.583322	3.217383
H	-0.222047	0.470626	2.192940
H	-1.083015	-3.797685	0.283953
O	-1.383579	-3.718933	-0.639369
H	-1.420046	-4.626383	-0.959277
H	-1.409646	-4.039098	2.518428
O	-0.564879	-4.037537	2.053609
H	-0.075423	-3.297534	2.446270
H	1.872019	-2.023185	2.891870
O	1.009096	-1.913259	3.316796
H	1.135292	-2.172052	4.240800
C	-2.440477	-1.346414	1.783926
H	-1.660887	-1.520789	2.526710
H	-2.932635	-2.293435	1.557879
H	-3.180197	-0.652247	2.187573
H	-1.684354	0.975540	-1.065071

G^*_{ZPE} = -687.64834 Hartrees

0 imaginary frequencies

Transition State

C	-1.878454	-0.230625	0.240224
C	-0.439104	-0.352491	0.026996
H	0.075410	-1.045532	0.689171
C	-2.728574	0.503409	-0.798672
H	-0.090750	-0.378547	-1.000933
O	-0.483039	0.993288	0.535690
O	-2.176911	1.511050	-1.454690
O	-3.859700	0.156915	-1.004150
H	0.964882	1.133063	3.169180
O	0.104002	0.756051	2.950845
H	0.178127	-0.209034	3.112931
H	-0.241568	0.966791	1.545220
H	-1.870925	-2.750875	-0.053628
O	-2.313286	-2.141924	-0.686513
H	-3.261070	-2.310868	-0.607826
H	-1.183718	-4.346183	1.501046
O	-0.819551	-3.545423	1.107762
H	-0.510002	-3.007709	1.858840
H	0.942358	-2.352562	3.633020
O	0.113382	-1.984036	3.302033
H	-0.530980	-2.153538	4.001437
C	-2.525412	-0.485533	1.552467
H	-1.892236	-1.099174	2.190779
H	-3.483328	-0.976522	1.375646
H	-2.739674	0.472090	2.034841
H	-1.318996	1.763795	-1.071129

G^*_{ZPE} = -687.61470 Hartrees

*i*563.91 cm^{-1}

Products

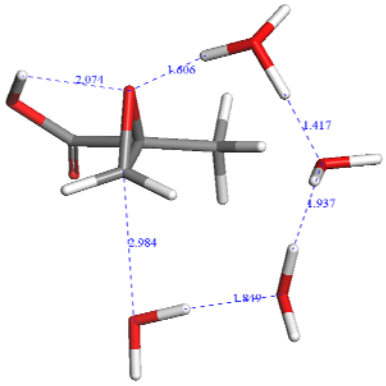
C	-2.142155	0.301511	-0.113099
C	-0.606537	0.298054	-0.109289
H	-0.274139	-0.551028	0.497011
C	-2.698696	1.410567	-1.005925
C	-2.723610	0.464455	1.288264
H	-0.243287	0.170858	-1.130593
O	-0.091128	1.517017	0.399294
O	-2.143108	2.608639	-0.869747
O	-3.623182	1.227187	-1.761953
H	-0.029873	1.424828	1.374823
O	-2.517197	-0.953824	-0.673181
H	-3.457487	-0.931460	-0.909819
H	0.925731	0.853381	3.378210
O	0.034625	0.818904	3.012077
H	-0.166861	-0.129058	2.933179
H	-2.152309	-2.119739	0.223898
H	-2.584271	-3.388138	1.143533
O	-1.820516	-2.882005	0.824290
H	-1.297171	-2.504922	1.643187
H	0.327660	-2.453499	2.826699
O	-0.527339	-2.002833	2.782973
H	-0.975129	-2.217138	3.613634
H	-3.814168	0.422323	1.245739
H	-2.423532	1.419676	1.722316
H	-2.353699	-0.346633	1.920129
H	-1.349580	2.542077	-0.287539

G^*_{ZPE} = -687.683.80 Hartrees

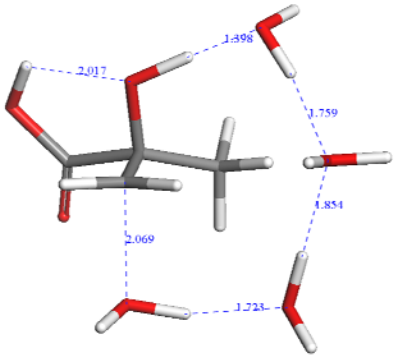
0 imaginary frequencies

16. MAE hydrolysis (H_3O^+, 3 H_2O) – nucleophile adds to primary carbon

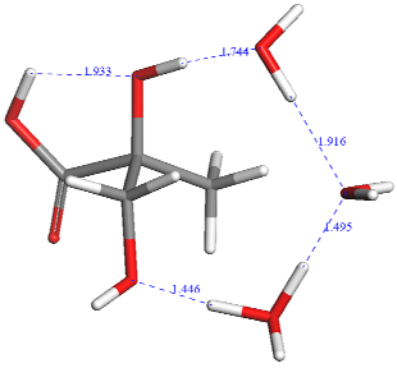
Reactants



Transition State



Products



Reactants

C	-1.469360	-0.758842	0.481793
C	-0.127323	-0.737833	-0.122275
C	1.045679	-1.406168	0.529271
H	-2.350422	-0.673293	-0.143376
H	-1.576928	-1.252555	1.442223
H	0.893727	-1.434861	1.609348
H	1.964843	-0.862443	0.302564
H	1.137011	-2.426519	0.154993
C	-0.074148	-0.601220	-1.623014
O	-0.659453	0.433909	0.517723
O	-0.671280	0.468406	-2.142888
O	0.462650	-1.421487	-2.324558
H	-0.989930	1.052765	-1.433616
H	-0.130419	0.748249	2.001120
O	-1.445273	-3.587550	-0.469161
H	-1.687829	-4.504452	-0.635478
H	1.028630	1.019964	3.074949
O	0.084891	0.813161	2.980854
H	-0.111043	-0.128467	3.425796
H	-1.118884	-3.584467	0.448838
H	-1.157096	-4.291909	2.683797
O	-0.554444	-3.711492	2.205198
H	-0.501773	-2.908250	2.747484
H	0.239211	-1.654752	4.632775
O	-0.414536	-1.403707	3.964687
H	-1.267068	-1.389213	4.422547

G^*_{ZPE} = -687.64831 Hartrees

0 imaginary frequencies

Transition State

C	-1.515200	-0.345109	0.121784
C	-0.147619	-0.416566	-0.379022
C	0.793979	-1.452238	0.170060
H	-2.257111	0.230929	-0.411828
H	-1.688809	-0.654954	1.144877
H	0.601588	-1.607232	1.232161
H	1.826705	-1.131731	0.021213
H	0.632519	-2.390015	-0.362987
C	-0.003193	-0.190764	-1.875986
O	-0.212767	0.845181	0.314105
O	-0.011080	1.071108	-2.284508
O	0.092595	-1.108697	-2.648879
H	-0.064073	1.671709	-1.520272
H	0.189400	0.774410	1.297857
O	-2.360295	-2.108723	-0.554387
H	-3.320278	-2.009886	-0.516336
H	1.561625	0.446309	2.648958
O	0.623888	0.677247	2.623404
H	0.144367	-0.087063	3.015554
H	-2.120429	-2.700021	0.197196
H	-2.070182	-4.035691	2.055775
O	-1.463961	-3.432589	1.611322
H	-1.256055	-2.745879	2.271652
H	-0.500559	-1.850335	4.305335
O	-0.874301	-1.429537	3.520462
H	-1.717859	-1.062066	3.814380

G^*_{ZPE} = -687.62296 Hartrees

*i*623.23 cm^{-1}

Products

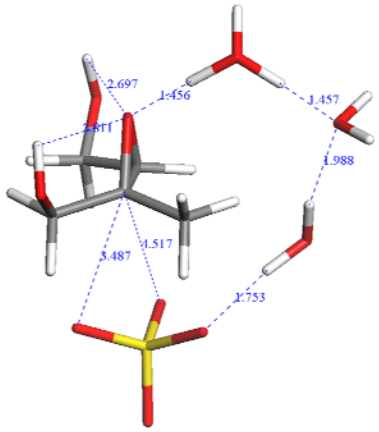
C	-1.608755	0.130654	-0.138517
C	-0.166500	-0.117490	-0.611714
C	0.330440	-1.501444	-0.221697
H	-1.976028	1.082498	-0.523823
H	-1.600050	0.161617	0.956155
H	0.313038	-1.590354	0.867551
H	1.353092	-1.641713	-0.576184
H	-0.302458	-2.278400	-0.651475
C	-0.126282	0.054763	-2.129456
O	0.640079	0.909066	-0.066624
O	0.341943	1.220716	-2.571345
O	-0.521212	-0.785513	-2.902012
H	0.642805	1.746868	-1.808467
H	0.585374	0.865151	0.914273
O	-2.463594	-0.931851	-0.575843
H	-3.342797	-0.582657	-0.769888
H	1.213327	0.620300	3.106507
O	0.375222	0.702605	2.637617
H	-0.091661	-0.134408	2.801987
H	-2.523008	-1.964411	0.434891
H	-3.369344	-2.866515	1.516554
O	-2.472956	-2.674595	1.200632
H	-1.912708	-2.304966	1.984872
H	-0.336798	-2.404664	3.262904
O	-1.045720	-1.772199	3.080341
H	-1.535652	-1.687106	3.909914

G^*_{ZPE} = -687.68105 Hartrees

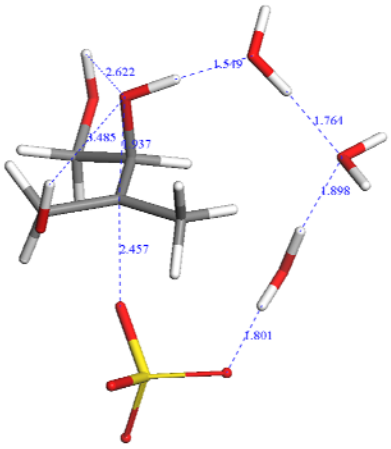
0 imaginary frequencies

17. β-IEPOX reaction with sulfate (H_3O^+, 2 H_2O, SO_4^{2-})

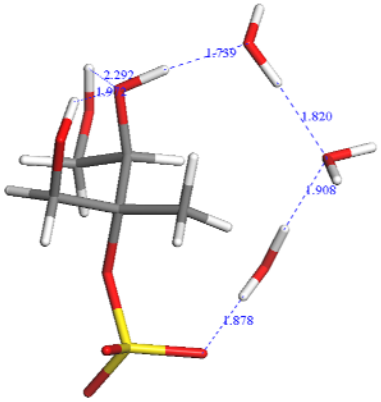
Reactants



Transition State



Products



Reactants			
C	-2.009447	-0.719267	0.672294
C	-0.790891	-1.358841	0.149745
H	-0.280907	-2.032269	0.837019
C	-3.072123	-0.163018	-0.243834
C	-0.410195	-1.537803	-1.292188
O	-0.752051	0.021931	0.607960
O	0.983707	-1.289093	-1.452010
O	-3.650260	1.017082	0.300161
H	-3.873876	-0.897665	-0.329257
H	-2.670241	0.036817	-1.237926
H	-0.989919	-0.885963	-1.947256
H	-0.586415	-2.575168	-1.573158
H	1.296032	0.781775	2.632793
O	0.427187	0.377061	2.779664
H	0.550690	-0.542900	3.252207
H	-0.047775	0.239698	1.863386
H	-1.049206	-4.121236	1.857689
O	-0.227954	-4.197349	2.386897
H	-0.094353	-3.336038	2.805403
H	1.580382	-2.095952	4.048221
O	0.659285	-1.848608	3.888766
H	0.228779	-1.864958	4.754336
C	-2.453240	-1.029977	2.076919
H	-1.640004	-1.487548	2.644819
H	-3.294916	-1.723704	2.047240
H	-2.774364	-0.116378	2.580965
H	-2.978548	1.709359	0.295579
H	1.141691	-0.354217	-1.274736
O	-1.162221	-4.873299	-0.886967
S	-2.567805	-4.551707	-0.472339
O	-2.571332	-4.174325	0.990423
O	-3.089840	-3.400127	-1.278141
O	-3.442611	-5.750903	-0.672880

G^*_{ZPE} = -1351.01885 Hartrees

0 imaginary frequencies

Transition State			
C	-2.077569	-0.191765	0.472201
C	-0.676660	-0.477334	0.121638
H	-0.228507	-1.259515	0.736247
C	-2.938461	0.609918	-0.448335
C	-0.208811	-0.551322	-1.309999
O	-0.447305	0.831140	0.686748
O	1.207805	-0.473595	-1.341759
O	-4.056195	1.191342	0.184620
H	-3.307826	-0.098737	-1.195106
H	-2.331076	1.358385	-0.962492
H	-0.653290	0.244202	-1.913613
H	-0.492870	-1.517146	-1.724651
H	1.249010	0.760659	3.238201
O	0.322829	0.524145	3.109809
H	0.264235	-0.432972	3.313181
H	-0.127565	0.729131	1.642251
H	-1.658224	-3.811350	1.353311
O	-0.692542	-3.926848	1.448808
H	-0.426788	-3.285376	2.125362
H	0.907312	-2.557723	3.956218
O	0.113114	-2.172550	3.565251
H	-0.591520	-2.356111	4.199596
C	-2.572435	-0.527383	1.819374
H	-1.882617	-1.172713	2.360992
H	-3.548043	-1.008652	1.702538
H	-2.755019	0.397438	2.375213
H	-3.754883	1.927487	0.731034
H	1.466202	0.410625	-1.056136
O	-4.147654	-4.176601	-1.106688
S	-3.803172	-3.101068	-0.129081
O	-3.450029	-3.716358	1.202016
O	-2.604989	-2.329067	-0.617933
O	-4.959968	-2.166268	0.042736

G^*_{ZPE} = -1351.00333 Hartrees

i 354.97 cm^{-1}

7 -- 21 bond distance fixed

22 -- 31 bond distance fixed

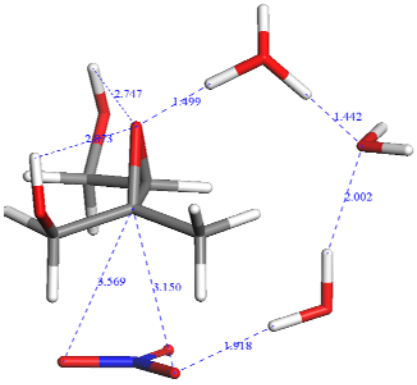
Products			
C	-2.353677	0.251273	0.176541
C	-0.824651	0.060259	0.046533
H	-0.533101	-0.789659	0.675944
C	-2.828935	1.590765	-0.411436
C	-2.750853	0.100552	1.636959
C	-0.335404	-0.205820	-1.369911
O	-0.160490	1.235757	0.502281
O	1.080932	-0.347100	-1.370683
O	-2.493967	2.702524	0.405718
H	-3.915986	1.565731	-0.485155
H	-2.419664	1.713684	-1.419449
H	-0.630718	0.611387	-2.037159
H	-0.746763	-1.138899	-1.749120
H	0.116377	1.091775	1.431666
H	1.532370	0.500738	3.086391
O	0.579533	0.639183	3.045242
H	0.188387	-0.240417	3.207169
H	-2.402829	-3.029745	0.978535
O	-1.501476	-3.344518	1.153575
H	-1.193144	-2.813671	1.905652
H	-0.129940	-2.423614	4.051796
O	-0.623331	-1.851355	3.451243
H	-1.456948	-1.673891	3.905293
H	-3.802289	0.340056	1.801083
H	-2.145730	0.786874	2.232938
H	-2.552158	-0.915971	1.976566
H	-1.540308	2.642970	0.562386
H	1.440587	0.431244	-0.927373
O	-5.311673	-0.434389	-0.151366
S	-4.349057	-1.492901	-0.472331
O	-2.899475	-0.784303	-0.694076
O	-4.156894	-2.455778	0.628534
O	-4.561804	-2.133535	-1.770600

G^*_{ZPE} = -1351.06183 Hartrees

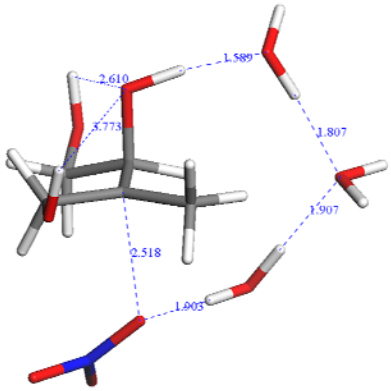
0 imaginary frequencies

18. β-IEPOX reaction with nitrate (H_3O^+, 2 H_2O, NO_3^-)

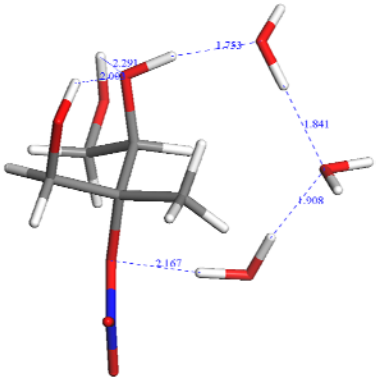
Reactants



Transition State



Products



Reactants			
C	-1.929720	-1.043776	0.497842
C	-0.482641	-1.325463	0.420275
H	-0.083241	-1.963784	1.208886
C	-2.716345	-0.629639	-0.722606
C	0.407747	-1.202972	-0.786946
O	-0.953383	-0.052739	0.934565
O	1.678964	-0.700322	-0.387690
O	-3.763725	0.269270	-0.382974
H	-3.186639	-1.521429	-1.140583
H	-2.067826	-0.185856	-1.479189
H	-0.032955	-0.557604	-1.547919
H	0.583878	-2.189204	-1.215514
H	-1.405685	-4.296254	1.511382
O	-1.018648	-4.526452	2.371464
H	-0.733803	-3.690884	2.767389
C	-2.739678	-1.616388	1.629756
H	-2.090166	-1.925217	2.449867
H	-3.307838	-2.478729	1.280100
H	-3.438683	-0.863529	1.999432
H	-3.365023	1.104611	-0.112430
H	1.567936	0.220194	-0.121860
N	-1.313333	-4.008636	-1.060385
O	-1.523579	-3.420786	-2.132748
O	-2.225019	-4.098811	-0.211391
O	-0.195872	-4.494083	-0.817933
H	0.391938	0.561446	3.536020
O	-0.422778	0.052256	3.401073
H	-0.251695	-0.940338	3.693161
H	0.874555	-2.527699	4.200718
O	-0.059905	-2.320474	4.062491
H	-0.499512	-2.524315	4.899524
H	-0.659854	0.066692	2.399610

G^*_{ZPE} = -932.10963 Hartrees

0 imaginary frequencies

Transition State			
C	-2.021339	-0.050280	0.381173
C	-0.610719	-0.469642	0.279584
H	-0.334589	-1.208191	1.032750
C	-2.666953	0.629009	-0.768279
C	0.003452	-0.796723	-1.062313
O	-0.262446	0.855998	0.712916
O	1.411616	-0.881062	-0.926406
O	-3.919863	1.198041	-0.478543
H	-2.816863	-0.147940	-1.530692
H	-1.966029	1.355989	-1.191931
H	-0.268194	-0.049857	-1.813226
H	-0.347287	-1.776989	-1.390482
H	-1.295909	-3.364469	0.764589
O	-0.611346	-3.799701	1.298041
H	-0.531774	-3.247620	2.092560
C	-2.727660	-0.165424	1.659980
H	-2.155223	-0.720116	2.400803
H	-3.682176	-0.660884	1.451761
H	-2.986329	0.834784	2.023461
H	-3.784633	2.015766	0.015290
H	1.745180	0.000346	-0.719427
N	-2.761051	-2.900285	-1.321033
O	-3.550782	-2.391597	-2.126521
O	-2.666526	-2.422690	-0.161558
O	-2.053932	-3.864074	-1.640945
H	1.064087	0.715564	3.515351
O	0.153581	0.541913	3.249354
H	0.005335	-0.409718	3.423102
H	0.240038	-2.582464	4.260938
O	-0.378069	-2.160285	3.651303
H	-1.234596	-2.206681	4.094666
H	-0.070540	0.807979	1.699148

G^*_{ZPE} = -932.08996 Hartrees

*i*255.44 cm^{-1}

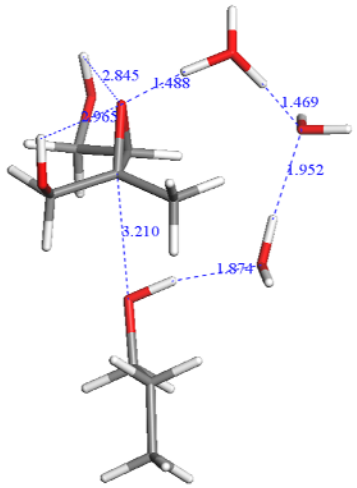
Products			
C	-2.284392	0.309050	-0.089755
C	-0.736019	0.220468	-0.075505
H	-0.444907	-0.526184	0.672643
C	-2.784251	1.537124	-0.870247
C	-2.808672	0.238100	1.336732
C	-0.097556	-0.161739	-1.406140
O	-0.219103	1.488385	0.300446
O	1.317344	-0.138165	-1.276654
O	-2.667603	2.718400	-0.095558
H	-3.841658	1.417462	-1.101561
H	-2.232536	1.628891	-1.810481
H	-0.416922	0.523649	-2.198334
H	-0.370792	-1.177883	-1.686353
H	0.028215	1.433925	1.247474
H	1.268043	0.867720	3.117991
O	0.332164	0.959890	2.907085
H	-0.035420	0.059502	2.989153
H	-1.568950	-2.581417	0.030906
O	-1.304380	-3.167298	0.749332
H	-1.126420	-2.577645	1.501261
H	-0.180640	-2.180302	3.690184
O	-0.735698	-1.638211	3.115732
H	-1.578164	-1.564747	3.581783
H	-3.829086	0.605222	1.427387
H	-2.164619	0.849631	1.972379
H	-2.756080	-0.794567	1.690981
H	-1.736119	2.788509	0.157875
H	1.554826	0.734389	-0.938205
N	-3.906717	-1.357686	-0.882167
O	-4.779802	-0.667794	-0.437970
O	-2.618121	-0.907402	-0.859186
O	-4.009997	-2.445650	-1.378781

G^*_{ZPE} = -932.12545 Hartrees

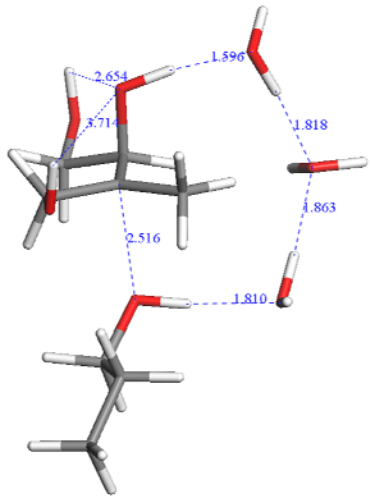
0 imaginary frequencies

19. β-IEPOX reaction with propanol (H_3O^+, 2 H_2O, $CH_3CH_2CH_2OH$)

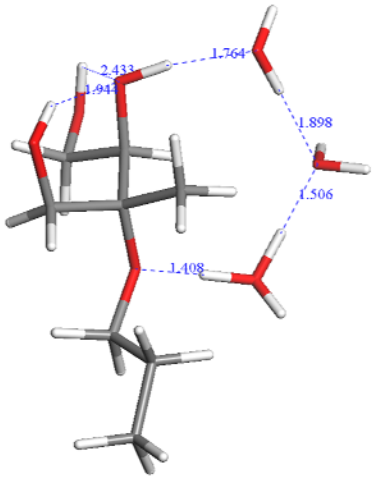
Reactants



Transition State



Products



Reactants

C	-1.738405	-0.386217	0.586253
C	-0.377227	-0.767129	0.182935
H	0.117320	-1.501129	0.818700
C	-2.711246	0.188499	-0.415666
C	0.215927	-0.645088	-1.190681
O	-0.604356	0.486854	0.882010
O	1.608861	-0.366951	-1.099101
O	-3.676832	1.025984	0.204761
H	-3.258875	-0.640890	-0.869104
H	-2.187252	0.734734	-1.200966
H	-0.285833	0.123420	-1.780042
H	0.116696	-1.603698	-1.700659
H	1.310943	0.681948	3.179897
O	0.463356	0.211241	3.143735
H	0.645342	-0.811561	3.205394
H	0.009670	0.403500	2.234774
H	-1.775871	-3.964999	2.148801
O	-0.933797	-3.995089	1.679496
H	-0.363003	-3.382524	2.170903
H	1.696029	-2.481760	2.808908
O	0.846841	-2.266398	3.219201
H	0.894879	-2.622965	4.116993
C	-2.356318	-1.029467	1.797135
H	-1.585543	-1.417460	2.464382
H	-2.999414	-1.853993	1.479191
H	-2.965873	-0.303988	2.338317
H	-3.229403	1.818483	0.523923
H	1.712069	0.533327	-0.769685
C	-5.147403	-5.072638	-0.399943
C	-4.064925	-4.029755	-0.140245
C	-2.874136	-4.229769	-1.063861
O	-1.866391	-3.236793	-0.885132
H	-4.758096	-6.083857	-0.253641
H	-5.518881	-5.001722	-1.425788
H	-5.995328	-4.938801	0.274118
H	-3.725924	-4.090351	0.899804
H	-4.464168	-3.021252	-0.291096
H	-3.195624	-4.161993	-2.106478
H	-2.446545	-5.228725	-0.913362
H	-1.484994	-3.369547	0.000882

G^*_{ZPE} = -845.89059 Hartrees

0 imaginary frequencies

Transition State

C	-1.803233	0.134271	0.423875
C	-0.404707	-0.150357	0.077616
H	0.035526	-0.950069	0.675633
C	-2.664035	0.863862	-0.546012
C	0.055968	-0.206058	-1.360564
O	-0.142069	1.143972	0.659995
O	1.473766	-0.192415	-1.400472
O	-3.879774	1.326406	-0.010099
H	-2.892805	0.140702	-1.339344
H	-2.086439	1.671624	-1.005107
H	-0.350488	0.628400	-1.937466
H	-0.276475	-1.142969	-1.805588
H	1.604151	0.752512	3.211704
O	0.681589	0.527727	3.042576
H	0.645978	-0.449935	3.041762
H	0.189385	0.993699	1.597862
H	-2.654734	-3.015230	2.580142
O	-1.942725	-3.425507	2.075493
H	-1.126102	-3.013594	2.412759
H	1.120291	-2.503862	2.184602
O	0.508314	-2.256850	2.889952
H	0.853270	-2.691013	3.680324
C	-2.312628	-0.155757	1.773589
H	-1.600542	-0.718775	2.372880
H	-3.246704	-0.713980	1.656325
H	-2.584213	0.784675	2.263154
H	-3.714669	2.141636	0.478750
H	1.773263	0.679616	-1.117227
C	-5.922861	-2.736979	-0.919829
C	-4.649367	-2.253337	-0.234334
C	-3.416717	-2.592643	-1.056368
O	-2.204551	-2.204486	-0.413070
H	-5.907478	-3.821845	-1.053695
H	-6.033814	-2.279846	-1.907083
H	-6.807953	-2.483149	-0.333572
H	-4.551370	-2.718430	0.753424
H	-4.689787	-1.170241	-0.081165
H	-3.442796	-2.066109	-2.015109
H	-3.392682	-3.668191	-1.270171
H	-2.141217	-2.679352	0.438741

G^*_{ZPE} = -845.87396 Hartrees

i318.44 cm^{-1}

Products

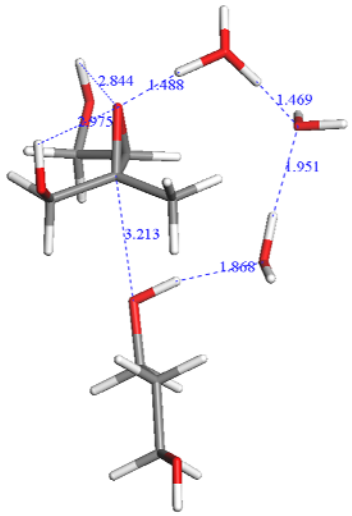
C	-2.149691	0.583591	0.064805
C	-0.613451	0.402157	-0.044195
H	-0.363419	-0.522623	0.494332
C	-2.655354	1.746220	-0.797235
C	-2.546535	0.747604	1.526967
C	-0.102785	0.287076	-1.469890
O	0.081513	1.495568	0.543792
O	1.268585	-0.092503	-1.474474
O	-2.092232	2.983421	-0.383052
H	-3.738094	1.843655	-0.692672
H	-2.430994	1.552167	-1.852015
H	-0.223554	1.246959	-1.984690
H	-0.648533	-0.480489	-2.017096
H	0.188977	1.312321	1.499626
H	1.229923	0.586662	3.423602
O	0.314301	0.644416	3.127727
H	0.026529	-0.278757	3.023539
H	-2.380162	-1.782437	0.365626
H	-3.003685	-2.911806	1.391838
O	-2.179869	-2.639576	0.957622
H	-1.486232	-2.415627	1.683604
H	0.390421	-2.528134	2.486726
O	-0.441468	-2.092612	2.719242
H	-0.690219	-2.456984	3.580017
H	-3.624923	0.866755	1.630154
H	-2.067401	1.631198	1.951004
H	-2.224804	-0.126321	2.100739
H	-1.174215	2.825216	-0.115571
H	1.750162	0.572097	-0.966808
C	-6.406291	-1.166409	-0.704995
C	-5.107793	-0.715286	-0.041395
C	-3.967330	-0.789948	-1.041448
O	-2.650567	-0.673053	-0.457606
H	-6.328950	-2.198944	-1.054811
H	-6.644570	-0.536557	-1.566357
H	-7.241613	-1.106681	-0.005598
H	-4.871502	-1.359126	0.812568
H	-5.219915	0.304435	0.333354
H	-4.075237	-0.050153	-1.836571
H	-3.948397	-1.777656	-1.507850

G^*_{ZPE} = -845.92227 Hartrees

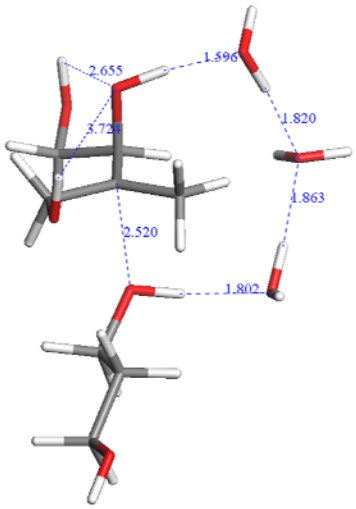
0 imaginary frequencies

20. β-IEPOX reaction with propane-1,4-diol (H_3O^+, 2 H_2O, $HOCH_2CH_2CH_2OH$)

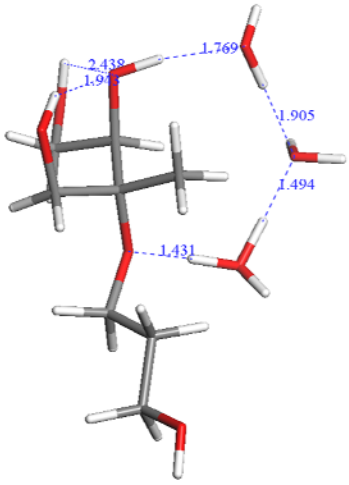
Reactants



Transition State



Products



Reactants

C	-1.745613	-0.397827	0.584756
C	-0.382525	-0.771625	0.181440
H	0.116011	-1.503141	0.816951
C	-2.721300	0.170860	-0.417963
C	0.209040	-0.646421	-1.192561
O	-0.615937	0.481115	0.880664
O	1.600095	-0.358873	-1.102233
O	-3.703626	0.987866	0.203376
H	-3.253435	-0.662541	-0.882385
H	-2.200383	0.731961	-1.194910
H	-0.298428	0.118154	-1.782203
H	0.115866	-1.605967	-1.701828
H	1.298216	0.683580	3.179073
O	0.451505	0.211267	3.143051
H	0.635696	-0.810940	3.205310
H	-0.002367	0.401694	2.233712
H	-1.769158	-3.976935	2.150537
O	-0.928454	-4.002978	1.678501
H	-0.359311	-3.387437	2.168168
H	1.693953	-2.477501	2.811768
O	0.842569	-2.265710	3.219365
H	0.889140	-2.622350	4.117217
C	-2.360107	-1.043817	1.795871
H	-1.587351	-1.429365	2.462165
H	-3.001126	-1.870168	1.478649
H	-2.971548	-0.320661	2.337987
H	-3.269729	1.781468	0.538212
H	1.697570	0.542023	-0.772778
C	-5.135934	-5.051993	-0.405888
C	-4.047339	-4.030660	-0.146254
C	-2.856549	-4.245729	-1.068428
O	-1.851544	-3.252915	-0.885980
H	-4.744970	-6.066311	-0.270587
H	-5.502545	-4.961249	-1.433878
O	-6.203079	-4.814835	0.514700
H	-3.721609	-4.107206	0.897033
H	-4.447046	-3.022816	-0.299930
H	-3.172417	-4.180510	-2.112339
H	-2.430934	-5.243697	-0.911344
H	-1.471853	-3.386135	0.001123
H	-6.909023	-5.441687	0.324934

G^*_{ZPE} = -921.11001 Hartrees

0 imaginary frequencies

Transition State

C	-1.811705	0.131856	0.425043
C	-0.411705	-0.146381	0.079197
H	0.033008	-0.941601	0.679891
C	-2.677145	0.849647	-0.548940
C	0.047081	-0.206307	-1.359513
O	-0.153780	1.151535	0.655300
O	1.464727	-0.189992	-1.401602
O	-3.899724	1.300226	-0.018710
H	-2.895362	0.122177	-1.341458
H	-2.106441	1.662082	-1.008634
H	-0.361849	0.625504	-1.938519
H	-0.284151	-1.145348	-1.801003
H	1.605070	0.774140	3.194940
O	0.680407	0.548997	3.038226
H	0.644892	-0.428626	3.041441
H	0.179545	1.006625	1.593344
H	-2.650423	-3.014498	2.597728
O	-1.935729	-3.420948	2.093748
H	-1.121593	-3.003208	2.429990
H	1.122238	-2.488468	2.193617
O	0.511324	-2.237734	2.898569
H	0.858855	-2.665830	3.691126
C	-2.318606	-0.154518	1.776135
H	-1.602033	-0.708549	2.378483
H	-3.248618	-0.720410	1.662157
H	-2.598279	0.786357	2.260324
H	-3.745720	2.118372	0.468843
H	1.762812	0.683347	-1.120941
C	-5.889695	-2.777099	-0.909752
C	-4.630630	-2.277810	-0.231089
C	-3.394351	-2.619168	-1.048901
O	-2.193046	-2.219181	-0.396819
H	-5.862328	-3.867684	-1.005432
H	-5.973441	-2.348931	-1.914769
O	-7.012833	-2.384730	-0.119040
H	-4.544096	-2.735607	0.761088
H	-4.695211	-1.192909	-0.098606
H	-3.415917	-2.097248	-2.009534
H	-3.362115	-3.695208	-1.256159
H	-2.131560	-2.689882	0.457989
H	-7.810652	-2.712849	-0.547043

G^*_{ZPE} = -921.09330 Hartrees

*i*314.92 cm^{-1}

Products

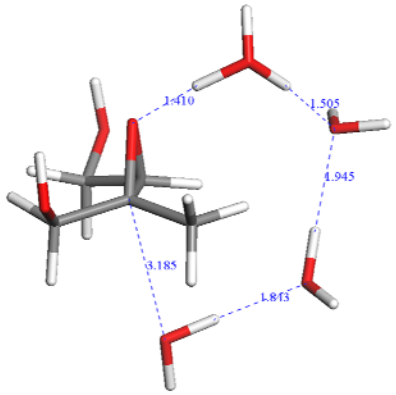
C	-2.126644	0.615885	0.035688
C	-0.593518	0.402503	-0.045382
H	-0.369972	-0.526443	0.496574
C	-2.591140	1.777542	-0.851534
C	-2.549757	0.812569	1.486708
C	-0.065260	0.278309	-1.464100
O	0.113984	1.481357	0.554675
O	1.299320	-0.124003	-1.452111
O	-2.002241	3.005794	-0.445882
H	-3.672252	1.904658	-0.764252
H	-2.356348	1.563890	-1.900229
H	-0.163586	1.239966	-1.980241
H	-0.617891	-0.479633	-2.018004
H	0.204382	1.290463	1.510518
H	1.209803	0.492912	3.422870
O	0.296222	0.584393	3.129390
H	-0.022536	-0.327360	3.017619
H	-2.462154	-1.753583	0.405166
H	-3.212391	-2.709653	1.505004
O	-2.367541	-2.587102	1.042783
H	-1.633654	-2.407219	1.746550
H	0.268074	-2.596194	2.454032
O	-0.539112	-2.137759	2.726645
H	-0.762734	-2.501451	3.594665
H	-3.628406	0.951123	1.564484
H	-2.064471	1.696099	1.903940
H	-2.253816	-0.055877	2.082200
H	-1.094865	2.827613	-0.154836
H	1.787020	0.536953	-0.945764
C	-6.366469	-1.154851	-0.748384
C	-5.102286	-0.607264	-0.113132
C	-3.943726	-0.729692	-1.091464
O	-2.643198	-0.640120	-0.475629
H	-6.243351	-2.220995	-0.968031
H	-6.577716	-0.633074	-1.688802
O	-7.442194	-0.965740	0.171999
H	-4.874746	-1.179100	0.792408
H	-5.267462	0.435203	0.170705
H	-4.015117	-0.000041	-1.899044
H	-3.941549	-1.724530	-1.542609
H	-8.230415	-1.374960	-0.200006

G^*_{ZPE} = -921.13985 Hartrees

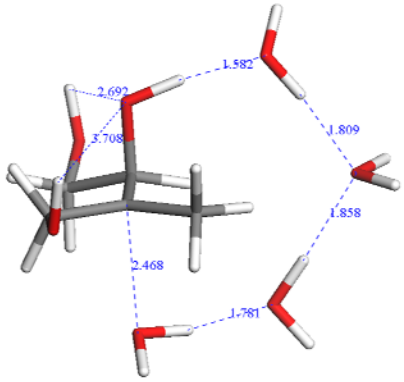
0 imaginary frequencies

21. β-IEPOX hydrolysis (ethanol continuum, H_3O^+, 3 H_2O)

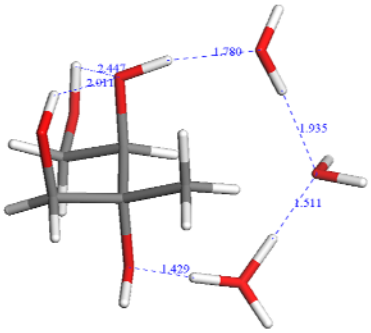
Reactants



Transition State



Products



Reactants			
C	-1.844545	-0.749099	0.463709
C	-0.442846	-1.023559	0.124145
H	0.094841	-1.674201	0.812626
C	-2.828046	-0.321993	-0.599257
C	0.177209	-0.925474	-1.239249
O	-0.803301	0.246539	0.740623
O	1.563326	-0.630606	-1.132207
O	-3.896600	0.435725	-0.055532
H	-3.267505	-1.224362	-1.030822
H	-2.326396	0.236241	-1.391378
H	-0.327329	-0.177365	-1.853319
H	0.093533	-1.898021	-1.726407
H	0.589023	1.089085	3.241320
O	-0.006544	0.341221	3.074712
H	0.492700	-0.544064	3.234076
H	-0.353976	0.361576	2.072619
H	-1.102102	-3.862317	0.367359
O	-1.512317	-3.763116	-0.510407
H	-1.521565	-4.652643	-0.878860
H	-1.018723	-4.375955	2.672674
O	-0.357507	-4.073486	2.039529
H	0.092367	-3.333574	2.477597
H	1.988527	-1.960141	2.995988
O	1.093025	-1.918209	3.360792
H	1.176745	-2.190608	4.285759
C	-2.440476	-1.370184	1.697132
H	-1.660677	-1.706562	2.382877
H	-3.048516	-2.231282	1.410348
H	-3.084112	-0.651508	2.207802
H	-3.560059	1.303159	0.197872
H	1.659691	0.289849	-0.862180

G^*_{ZPE} = -728.08270 Hartrees

0 imaginary frequencies

Transition State			
C	-1.885084	0.003651	0.202233
C	-0.462405	-0.297517	-0.008633
H	-0.078296	-1.060810	0.670301
C	-2.645278	0.735393	-0.851285
C	0.113078	-0.451475	-1.396780
O	-0.243967	1.025347	0.518216
O	1.527394	-0.451596	-1.323676
O	-3.902072	1.198873	-0.430435
H	-2.800292	0.018320	-1.664744
H	-2.018658	1.541359	-1.244588
H	-0.239740	0.341992	-2.061942
H	-0.195804	-1.416651	-1.799165
H	1.208569	0.932379	3.284519
O	0.334167	0.634748	3.006595
H	0.292880	-0.319139	3.216214
H	0.010086	0.937626	1.488126
H	-1.927725	-2.802623	0.008528
O	-2.401841	-2.254927	-0.648266
H	-3.334335	-2.477191	-0.546778
H	-0.971137	-4.450481	1.467351
O	-0.821863	-3.538515	1.194511
H	-0.540995	-3.065414	1.997909
H	0.899339	-2.496669	3.736680
O	0.063244	-2.096619	3.463520
H	-0.533327	-2.232415	4.211523
C	-2.505726	-0.250127	1.514500
H	-1.879362	-0.875346	2.149917
H	-3.477075	-0.720687	1.340966
H	-2.718021	0.707389	2.001951
H	-3.787089	2.020070	0.062270
H	1.823248	0.439892	-1.104341

G^*_{ZPE} = -728.06772 Hartrees

*i*333.94 cm^{-1}

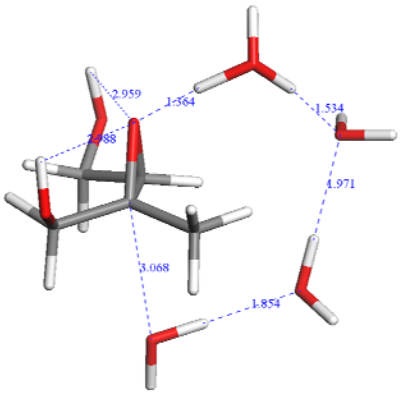
Products			
C	-2.168652	0.351345	-0.088489
C	-0.625934	0.351133	-0.058686
H	-0.302256	-0.494235	0.565291
C	-2.745949	1.423858	-1.018812
C	-2.740161	0.459290	1.315618
C	0.028924	0.212284	-1.422849
O	-0.147704	1.566024	0.503044
O	1.431897	0.041747	-1.279314
O	-2.483359	2.738364	-0.560058
H	-3.833127	1.306482	-1.049871
H	-2.364524	1.276293	-2.035103
H	-0.180216	1.101271	-2.028434
H	-0.347911	-0.667638	-1.944707
H	-0.081779	1.445587	1.471222
O	-2.527126	-0.933870	-0.653687
H	-3.485980	-0.972769	-0.791671
H	0.823633	0.884235	3.574059
O	-0.020686	0.778512	3.120901
H	-0.164483	-0.179955	3.063371
H	-2.123471	-2.041067	0.155318
H	-2.495801	-3.432862	0.986123
O	-1.764830	-2.845071	0.737536
H	-1.279546	-2.524258	1.585700
H	0.356371	-2.493879	2.822262
O	-0.511775	-2.065469	2.803499
H	-0.953767	-2.345519	3.617925
H	-3.830248	0.381804	1.277036
H	-2.480490	1.415962	1.770840
H	-2.348195	-0.344113	1.945268
H	-1.560903	2.771450	-0.266523
H	1.771728	0.817292	-0.816520

G^*_{ZPE} = -728.11281 Hartrees

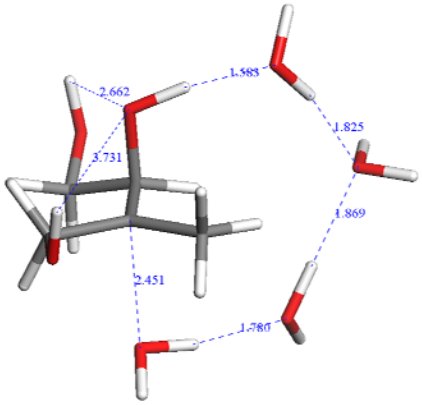
0 imaginary frequencies

22. β-IEPOX hydrolysis (1-octanol continuum, H_3O^+, 3 H_2O)

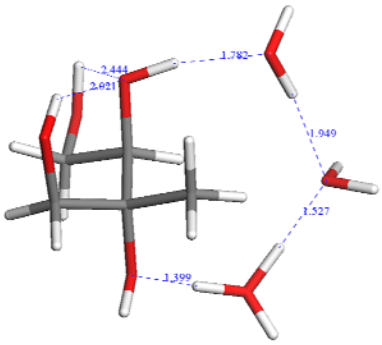
Reactants



Transition State



Products



Reactants

C	-1.826024	-0.769143	0.481995
C	-0.422855	-1.024445	0.140973
H	0.129504	-1.650685	0.840467
C	-2.822034	-0.370605	-0.579756
C	0.195965	-0.944774	-1.223795
O	-0.797780	0.255261	0.736000
O	1.573951	-0.615913	-1.118617
O	-3.884201	0.397431	-0.041837
H	-3.261644	-1.286049	-0.981842
H	-2.330498	0.166868	-1.392413
H	-0.324531	-0.226023	-1.859053
H	0.132489	-1.932293	-1.682998
H	0.624660	1.139717	3.180770
O	0.017975	0.397612	3.034118
H	0.488278	-0.486227	3.231550
H	-0.352937	0.389733	2.018239
H	-1.167241	-3.811811	0.326930
O	-1.606313	-3.658317	-0.527495
H	-1.616261	-4.518824	-0.958696
H	-0.906492	-4.537895	2.595656
O	-0.346974	-4.064418	1.970328
H	0.046330	-3.336538	2.474900
H	1.947752	-2.006858	3.086553
O	1.038413	-1.907872	3.401978
H	1.055604	-2.179269	4.330781
C	-2.403360	-1.375262	1.730942
H	-1.613086	-1.669154	2.424580
H	-2.981065	-2.262734	1.463397
H	-3.071218	-0.665367	2.221837
H	-3.549995	1.274572	0.176991
H	1.651433	0.324358	-0.922539

G^*_{ZPE} = -728.07001 Hartrees

0 imaginary frequencies

Transition State

C	-1.924842	0.006508	0.213233
C	-0.505100	-0.329401	0.065389
H	-0.159557	-1.079365	0.780095
C	-2.633028	0.727829	-0.885774
C	0.122400	-0.533123	-1.294379
O	-0.278609	1.005790	0.558507
O	1.531701	-0.514490	-1.167429
O	-3.903383	1.203883	-0.526738
H	-2.757665	0.001875	-1.696019
H	-1.984225	1.525253	-1.260595
H	-0.212357	0.227439	-2.005561
H	-0.162306	-1.516276	-1.669374
H	0.871683	1.142402	3.493471
O	0.148547	0.655847	3.080843
H	0.313195	-0.289519	3.261158
H	-0.074112	0.947157	1.541282
H	-2.044783	-2.804560	0.070190
O	-2.451874	-2.239658	-0.615419
H	-3.385152	-2.480015	-0.632942
H	-0.673302	-4.390797	1.211684
O	-1.134861	-3.565848	1.396860
H	-0.580713	-3.088313	2.037727
H	1.312113	-2.387408	3.210764
O	0.390425	-2.112264	3.301074
H	0.119741	-2.428364	4.173008
C	-2.600369	-0.193381	1.508079
H	-2.012088	-0.803404	2.191262
H	-3.572054	-0.654226	1.312577
H	-2.814774	0.782315	1.956533
H	-3.809448	2.040747	-0.057340
H	1.809401	0.388396	-0.973340

G^*_{ZPE} = -728.05748 Hartrees

i 338.86 cm^{-1}

i 18.12 cm^{-1}

7 -- 24 bond distance fixed

Products

C	-2.165997	0.348428	-0.088413
C	-0.623401	0.346843	-0.061846
H	-0.297300	-0.501110	0.558612
C	-2.745113	1.421668	-1.016463
C	-2.735750	0.454029	1.315833
C	0.031918	0.209441	-1.426316
O	-0.145447	1.560125	0.499218
O	1.433644	0.043928	-1.279413
O	-2.491374	2.732936	-0.550974
H	-3.831986	1.300259	-1.050528
H	-2.361485	1.278937	-2.032744
H	-0.180430	1.097317	-2.032275
H	-0.341341	-0.671735	-1.948710
H	-0.084056	1.444304	1.467745
O	-2.526679	-0.938713	-0.655361
H	-3.479312	-0.964098	-0.832123
H	0.804439	0.929025	3.594718
O	-0.019570	0.777535	3.118620
H	-0.131319	-0.185134	3.087281
H	-2.145927	-2.020723	0.145391
H	-2.508334	-3.435796	0.977223
O	-1.788793	-2.829189	0.743368
H	-1.304157	-2.521351	1.590574
H	0.358802	-2.511591	2.814528
O	-0.506857	-2.078015	2.815301
H	-0.929757	-2.349024	3.642436
H	-3.825831	0.375423	1.281088
H	-2.478255	1.411715	1.769679
H	-2.340785	-0.345774	1.948364
H	-1.566736	2.775510	-0.266491
H	1.770870	0.827055	-0.828031

G^*_{ZPE} = -728.09922 Hartrees

0 imaginary frequencies